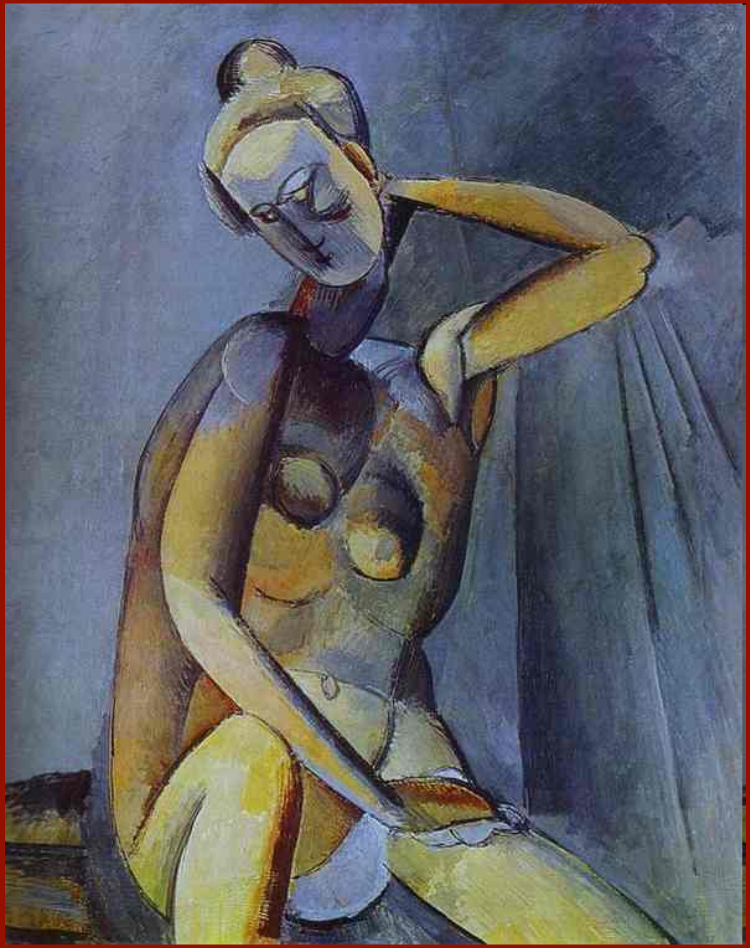
modeling the ocean ?can/should we move from bgc to ecology?



cosimo solidoro
csolidoro@inogs.it

NATURE IS COMPLEX
AND FULL OF DETAILS WHICH MAKE A DIFFERENCE

CAN WE STILL AFFORD TO MODEL IT AS 50 YEARS AGO?
(AS FIRST ORDER KINETIC CHEMICALS ?)

DO WE KNOW ANY BETTER?
CAN WE AFFORD MORE COMPLEX REPRESENTATION?
IS THIS WORTH ?

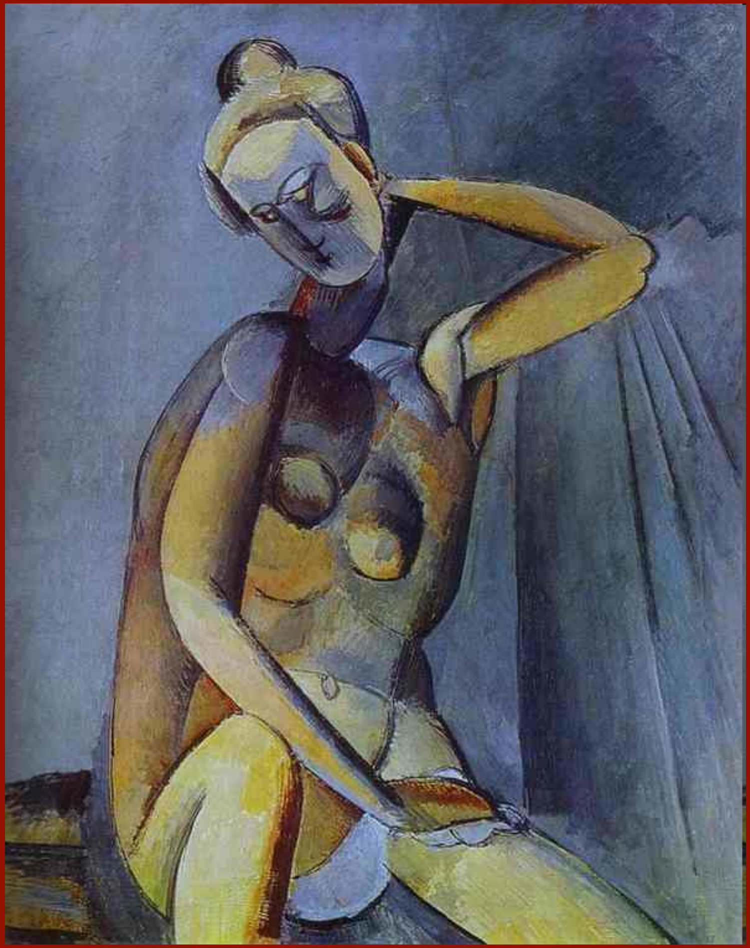
two words about MODELS……

Knowledge, in every field, is the result of a number of steps:

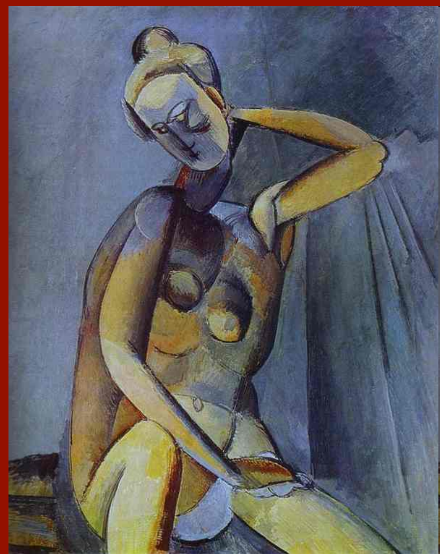
- gathering of *empirical* information, also through collection *direct observation*
- *empirical* understanding of phenomena (i.e. identification of relationships among vairables).
- *theoretical* understanding of relationships among vairables, (hypothesis of cause- effect mechanisms, identification of conceptual models, *quantitative* understanding of phenomena (set up of a THEORY)
- collection new data for *corroboration /falsification* model
- application of the model to new problems

a model is an ideal representation of selected aspects of reality

"Art is a lie that helps us to realize the truth". (picasso)



a model captures selected essential features/particular aspects of reality.



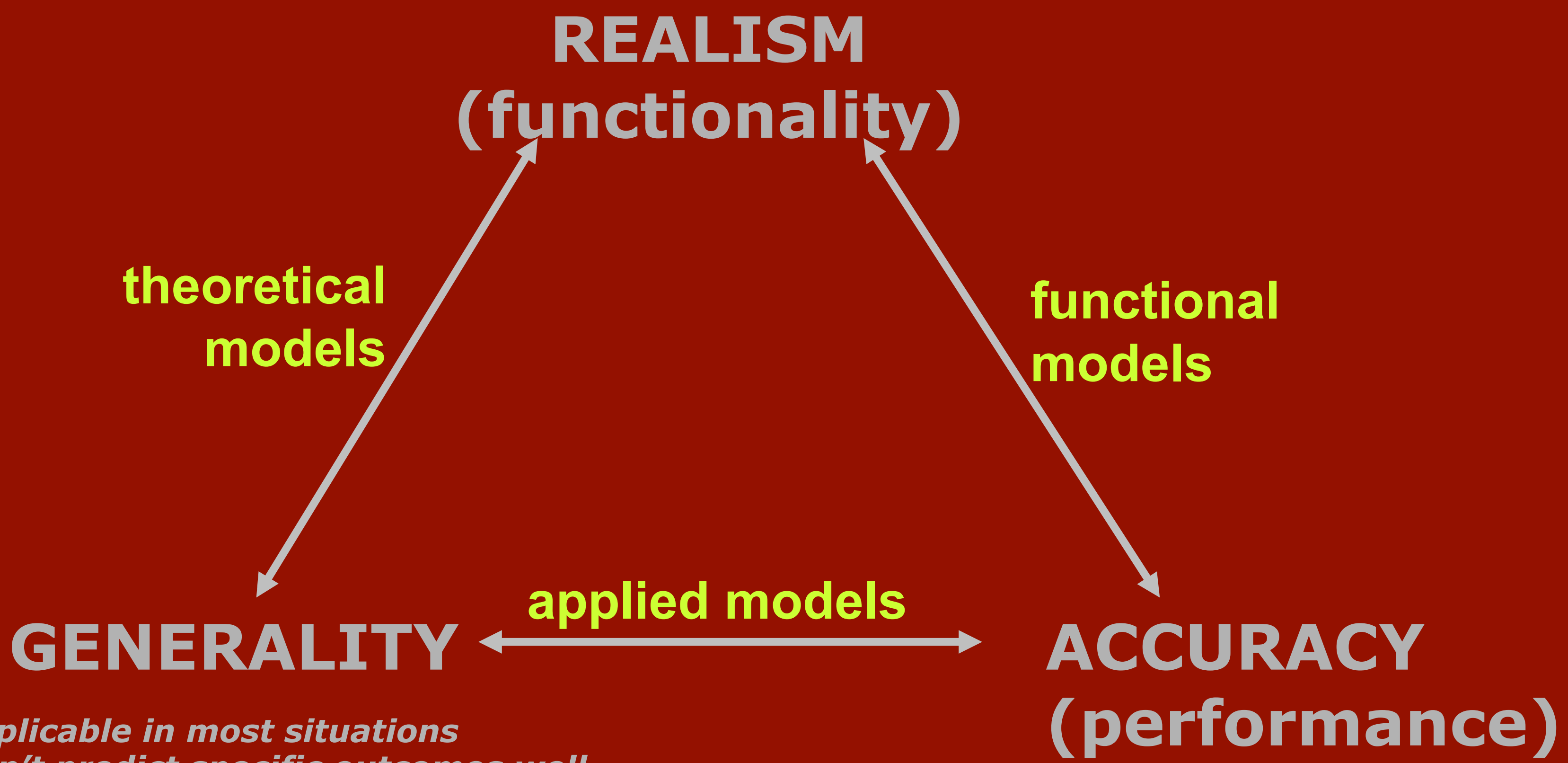
"Art is a lie that helps us to realize the truth".
(picasso)

WHERE IS REALITY ??
THERE IS NO REALITY
(nor real women) just cartoon

…e "reality" there can be different
…models….
ALL 'wrong' , 'difunctional' and 'incomplete'

2) A model would serve for certain purposes but not for others

Account for known relationships
May be complex

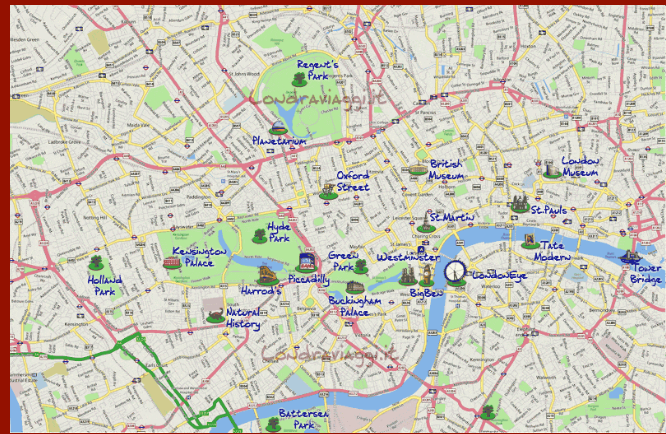


Applicable in most situations
Don't predict specific outcomes well
Typically "simple"
Good for exploring relationships

Accurately describe specific situations
May perform worse in other situations
Typically detailed

Modified from Levins (1968)

the 'best' london map ?



You do not need to know (consider) everything to learn something

Every model is 'difunctional' to some degree:

(the only perfectly representation of nature is nature)

When you go sailing you assume the earth is at the center of the universe..

NPD ocean model assumed zooplankton makes phtosysynthesis ….

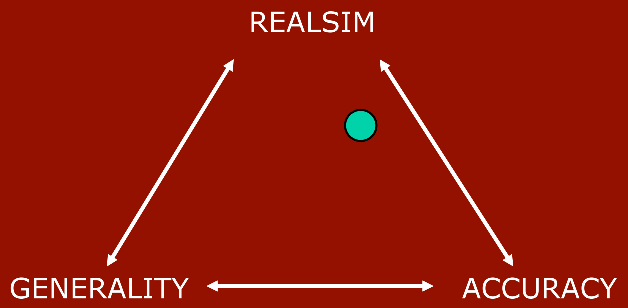
ocean models usually are:

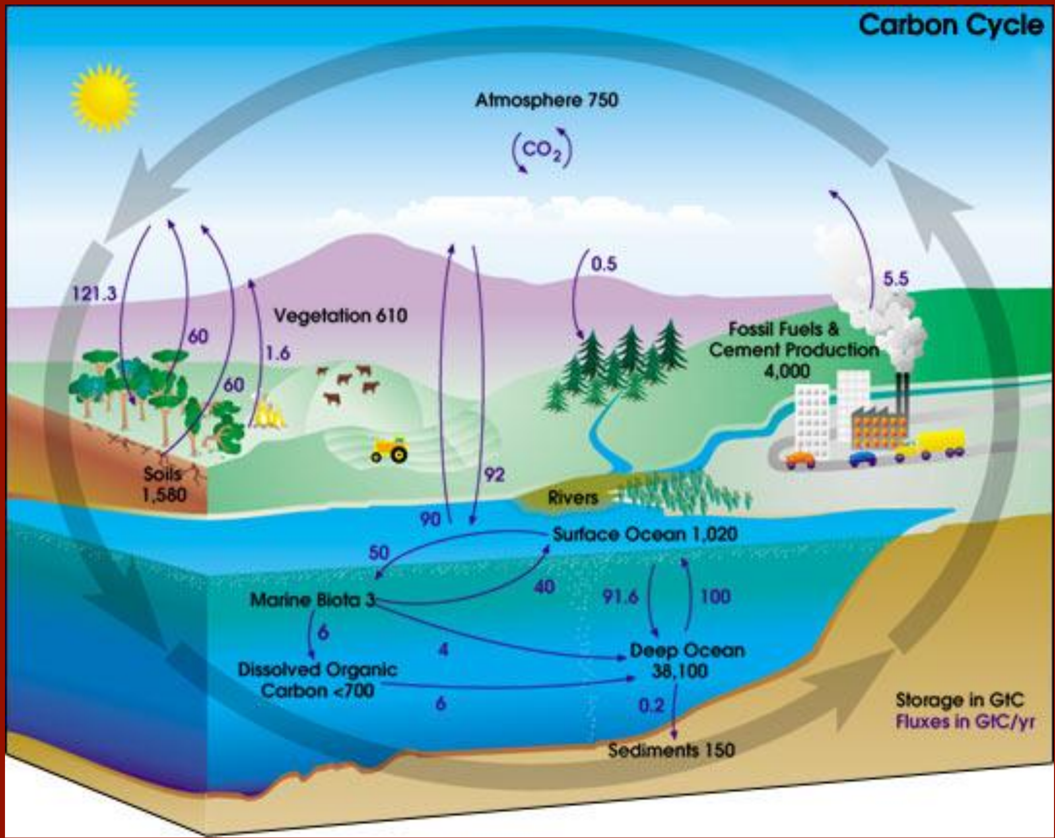
deterministic

process oriented

(simple),

spatially resolved (coupled to transport models)





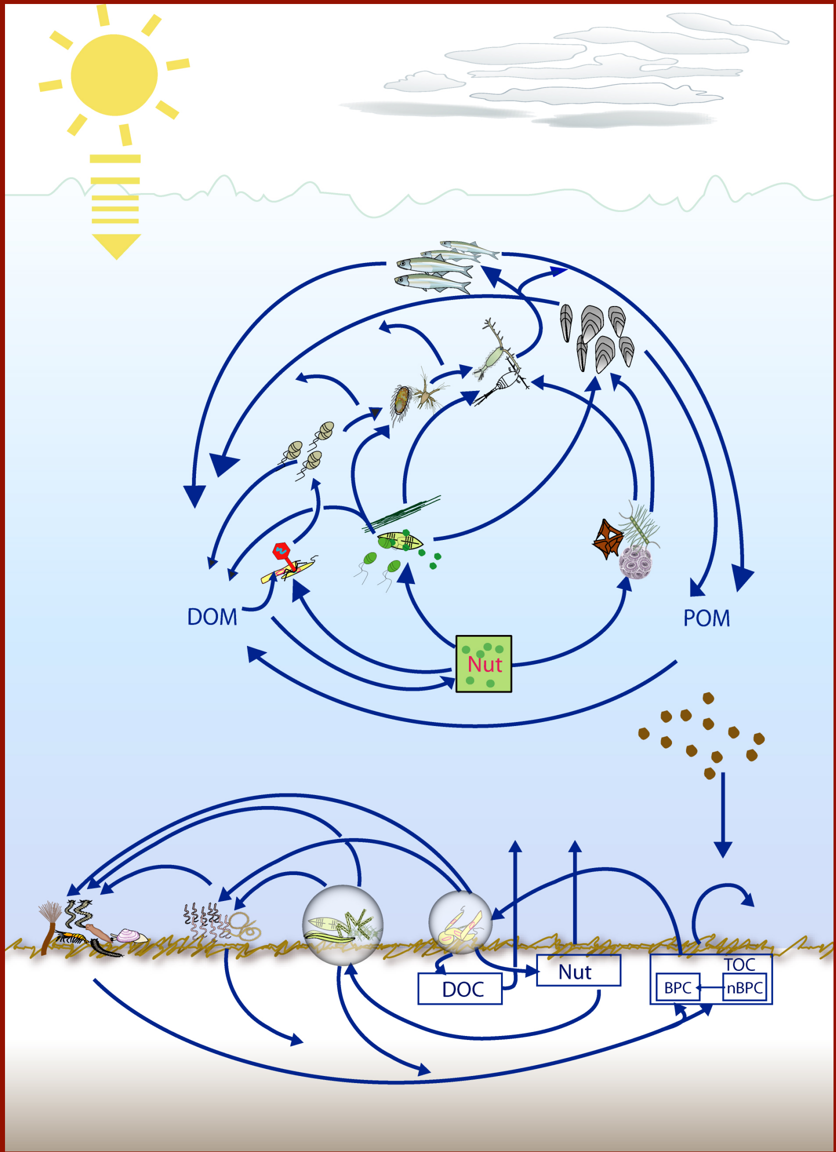
Streeter and phelps (1927)

jorgensen (1976)
nyholm (1974)

riley (1958)
fasham (1993)
baretta et al. (1996)

Biogeochemical models quantitatively describes element(s) (chem) flux(es) through biotoic (bio) and abiotic (geo) phases, As a function of external conditions.

http://earthobservatory.nasa.gov/Library/CarbonCycle/carbon_cycle4.html



Focus on NUTIRENTs rather than on ORGANISMs

Chemisrty rather than biology

Biogeochemical cycles:

Nut-> plancton ->
-> pesci -> detrito-
-> disciolto -> nutriente

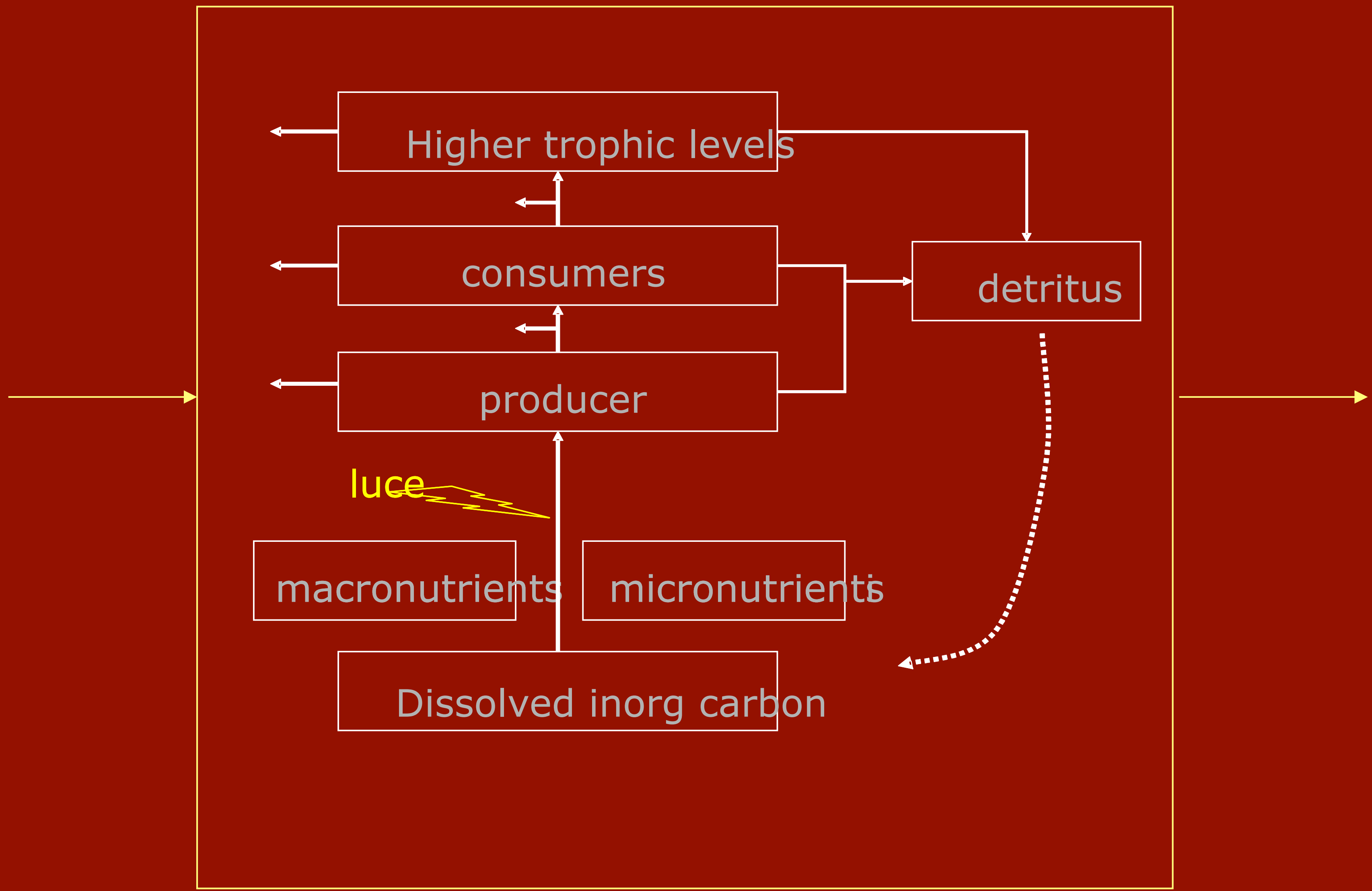
..+ benthic-pelagic processes …

DETERMINISTIC MODELS

Basic idea:

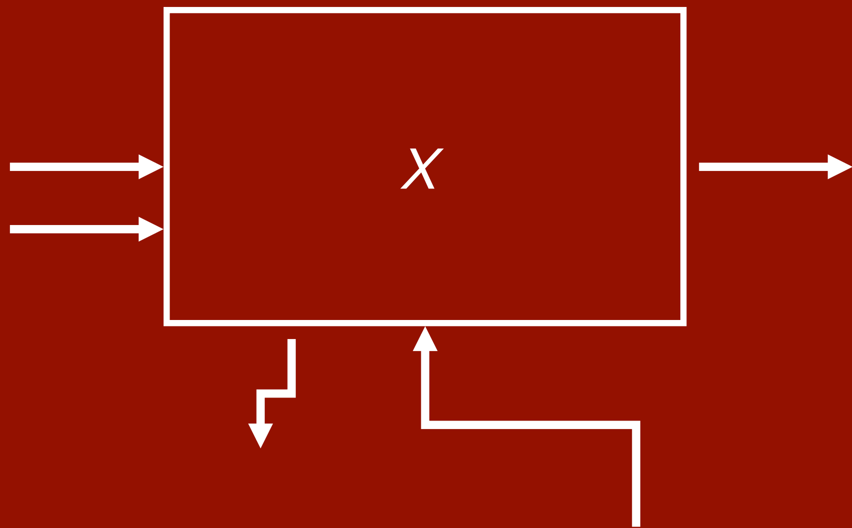
1. a *system (*the piece of reality we are interested in) can be efficiently described by a finite number of variables (*state variables*),

2. both the system and its evolution in time can be explained as a function of interactions (input, boundary conditions, controls) among the system and the remaining part of the universe


Higher trophic levels
consumers
detritus
producer
luce
macronutrients
micronutrients
Dissolved inorg carbon

Per ogni comparto posso fare 'bilancio' (somma analitica flussi) ..

$$\frac{dX}{dt} = sources - sinks$$



Biogeochemical flux Model

Set of Advection-Diffusion-Reaction equations:
Conservation laws with source and sink terms

$$\frac{\partial c}{\partial t} = \left.\frac{\partial c}{\partial t}\right|_{phys} + \left.\frac{\partial c}{\partial t}\right|_{bio}$$

$$\frac{\partial c}{\partial t} = A_{phys}(c) + D_{phys}(c) + R_{bio}(c)$$

Linear transport term

Non linear reaction term

physics

biology

Coupling hydrodynamical and biological modules

$$\frac{\partial \Theta_i}{} = -U \cdot \nabla \Theta_i + \nabla$$

generic passive tracer

$$\frac{\partial \Theta_i}{\partial t} = -U \cdot \nabla \Theta_i + \nabla \left[k \nabla \Theta_i - < u' \theta' > \right] + q \left(\Theta + \theta', \overline{T} + T', \overline{I} + I', .. \right)$$

generic active tracer

$$\frac{\partial \Theta_i}{} = -U \cdot \nabla \Theta_i + \nabla \left[k \nabla \Theta_i \right.$$

proper time scale (x-y vs z; biology “slow”)

$$\frac{\partial \Theta_i}{\partial t} = -U \cdot \nabla \Theta_i + k_h \nabla_H^2 \Theta_i + \frac{\partial}{\partial z} \left[K_v \frac{\partial \Theta_i}{\partial z} \right] + w_{si} \frac{\partial \Theta_i}{\partial z} + q \left(\Theta, \overline{T}, \overline{I}, .. \right)$$

standard formulation

0D application

$$\frac{\partial \Theta_i}{\partial t} = q\left(\Theta, \bar{T}, \bar{I}, ..\right)$$

(Rinaldi, Gatto, ….)

'toys model' ma anche applicazioni

orrizont. omogeno 1D

$$\frac{\partial \Theta_i}{\ } = \frac{\partial}{\ }\left[K \frac{\partial \Theta_i}{\ }\right] + \ldots$$

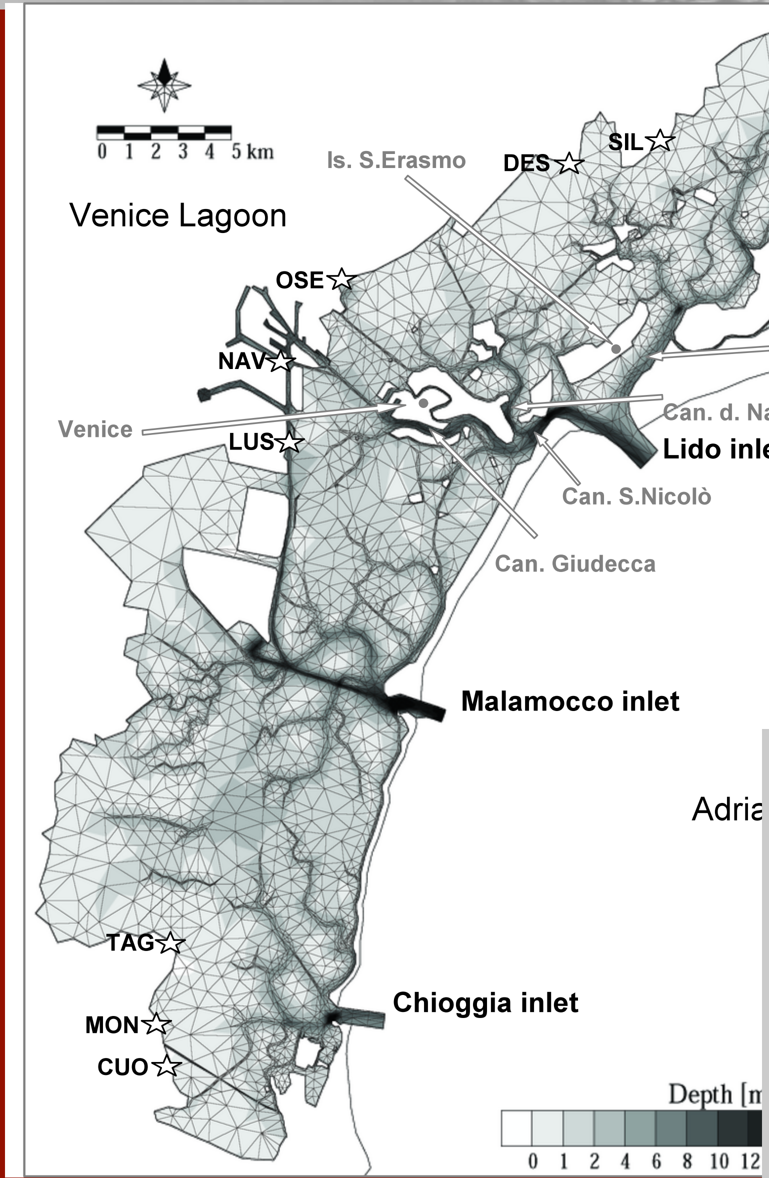
(many ! DCM jamart,77, varela 92,94)

'process oriented model'

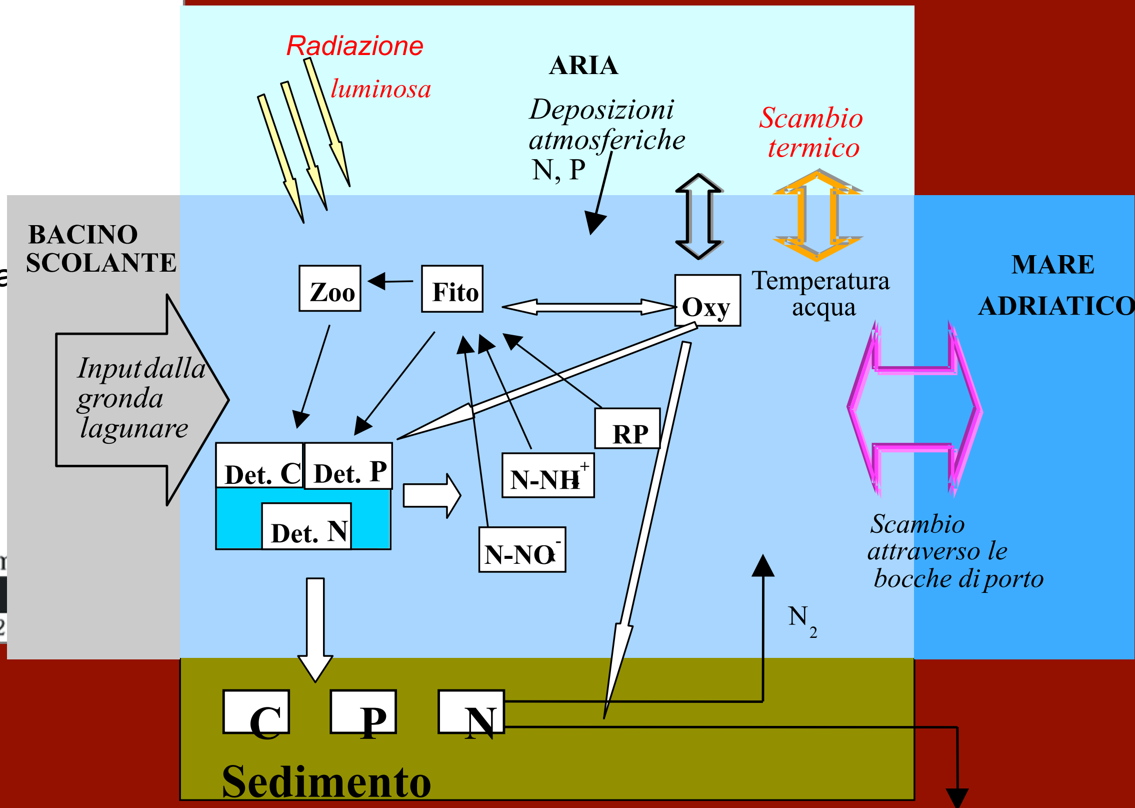
vert. omogeno 2D

$$\frac{\partial \Theta_i}{\partial t} = -U \cdot \nabla \Theta_i + k_h \nabla_H^2 \Theta_i + q\left(\Theta, \bar{T}, \bar{I}, ..\right)$$

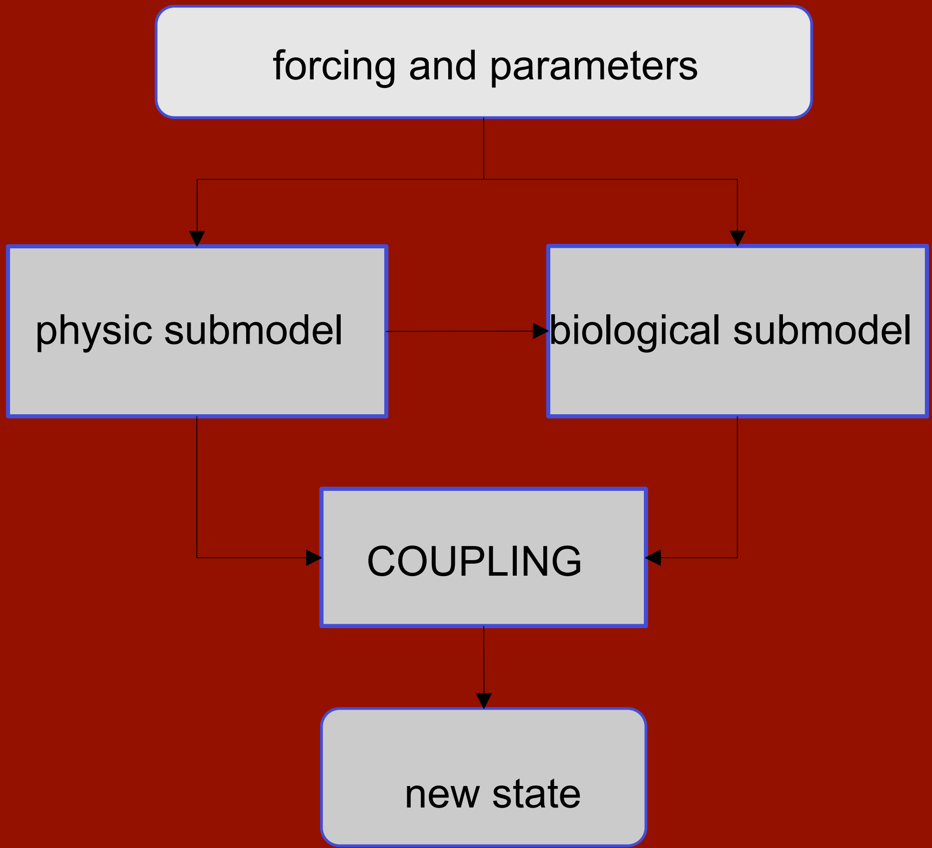
(not very frequent)



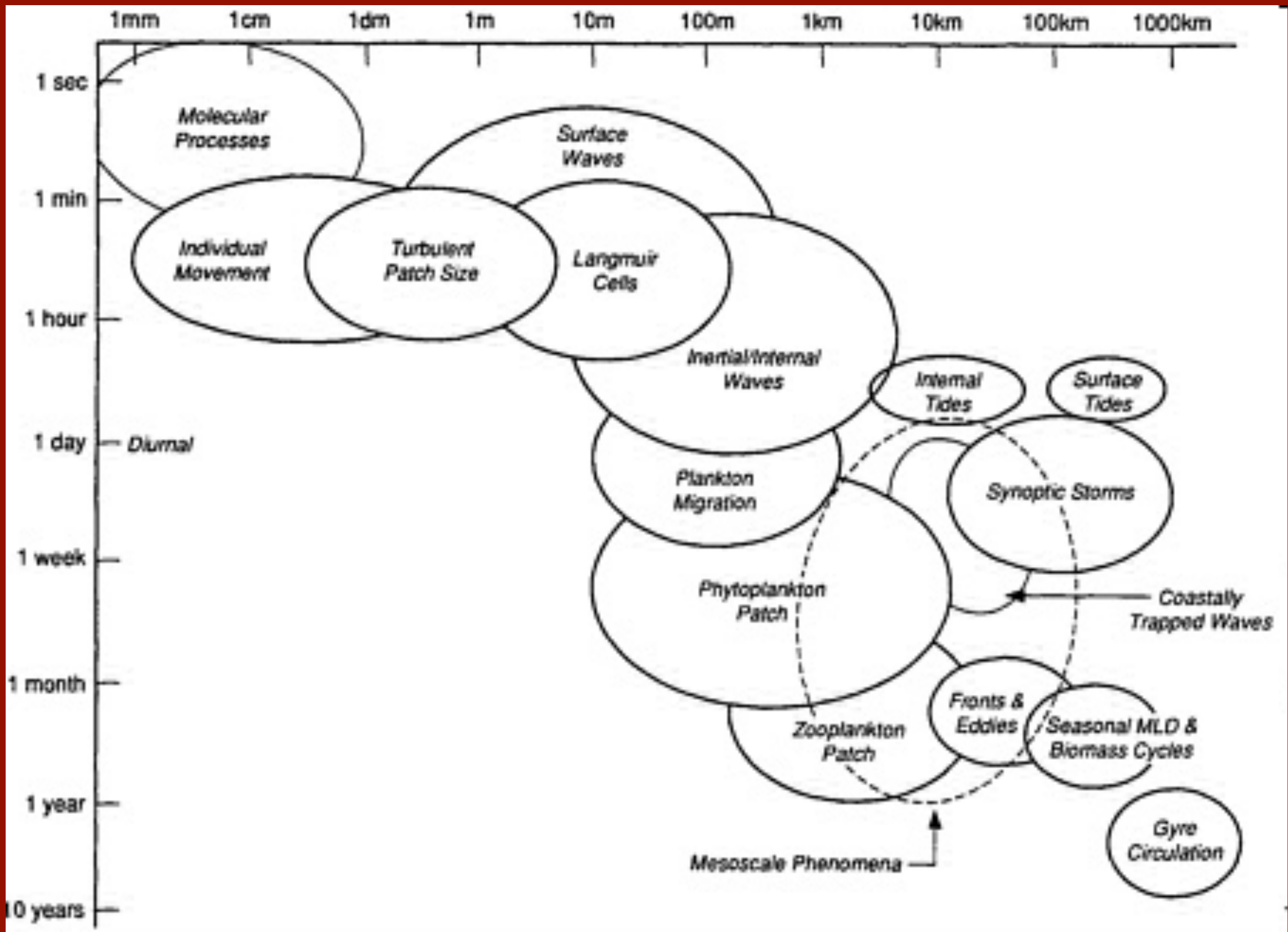
$$\frac{\partial c}{\partial t} = A_{phys}(c) + D_{phys}(c) + R_{bio}(c)$$



Numerical Integration



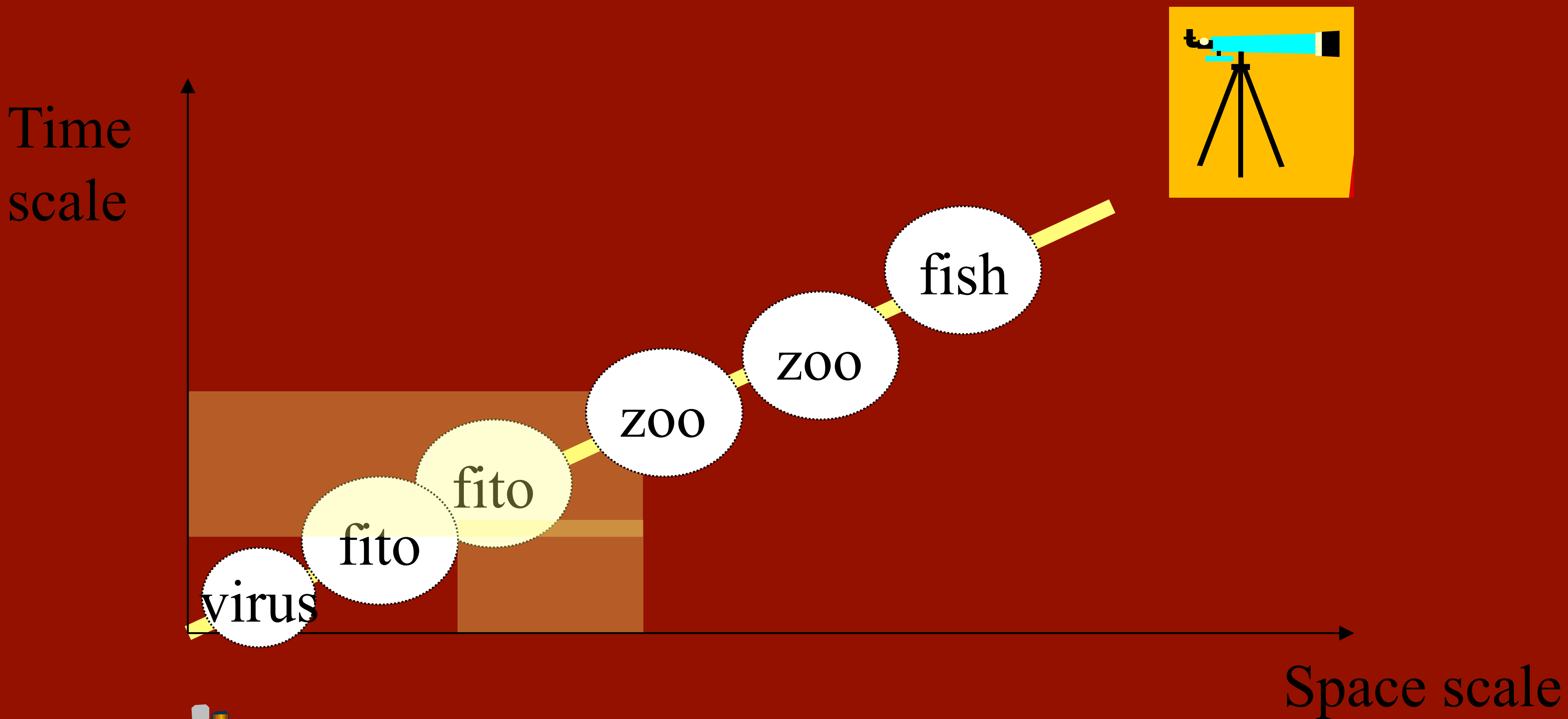
Operator splitting technique: forcings and parameters are input for each of the two subsystems for the derivative computation in the proper time step. The derivatives are coupled afterwards, allowing different time steps for the two processes and therefore optimising the computational resources

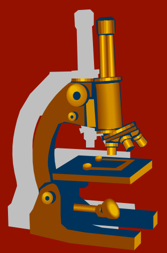


1-10 years

100m – 50 km

Dickey 2001





Subgrid parameterization=
closure= details not explicitly considered,
their effects 'somehow' included

reductionstic
(mechaniscistic?)

whole= sum of parts

the higher the number
of details the better
System description

systemic (holistic)

Whole <> sum of parts

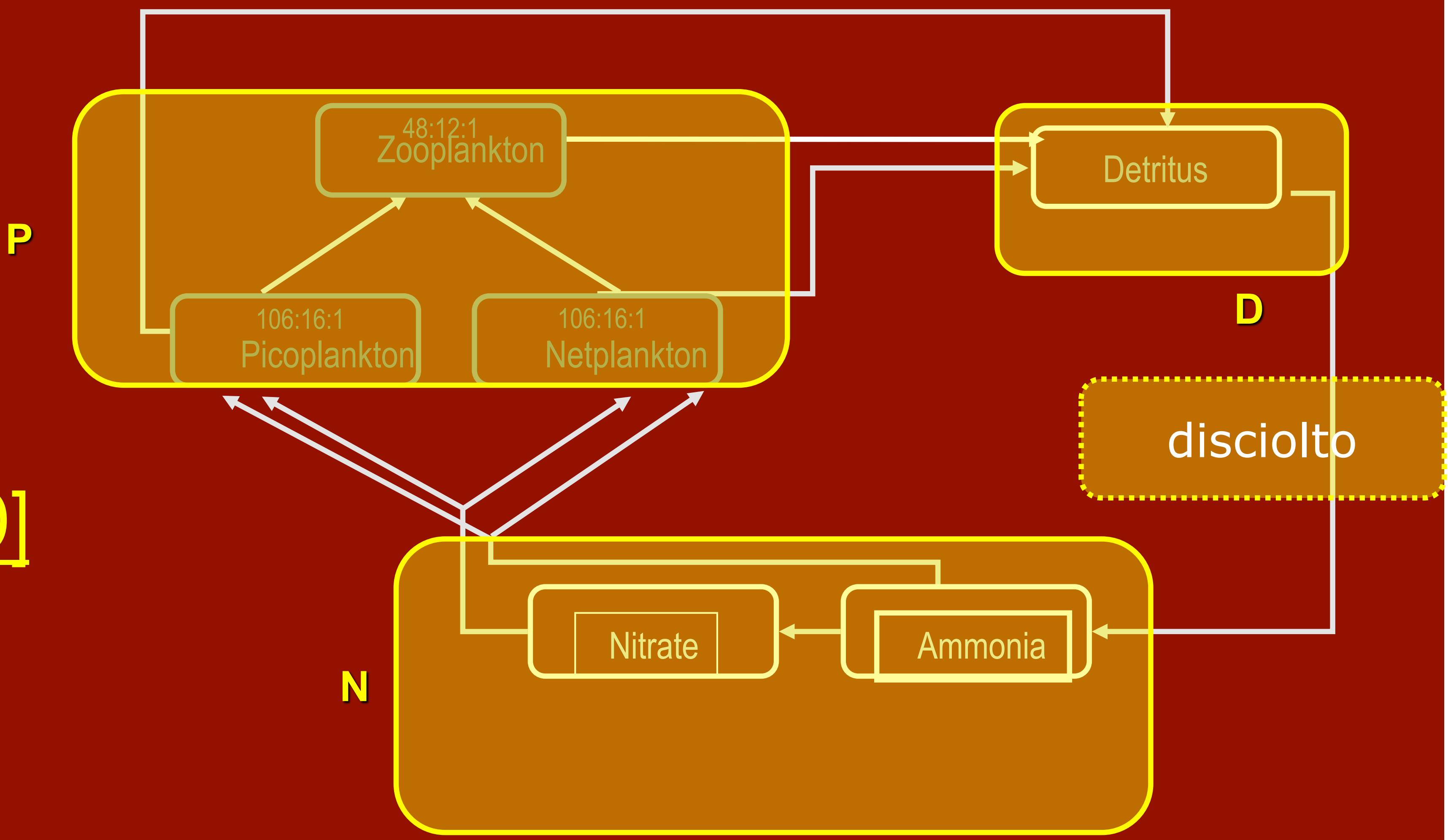
every descrition is an
approximation
Focus on selected details
only and paremetrize
what is left out

modelers can't be (only)
reductionistics

The BIOLOGICAL term

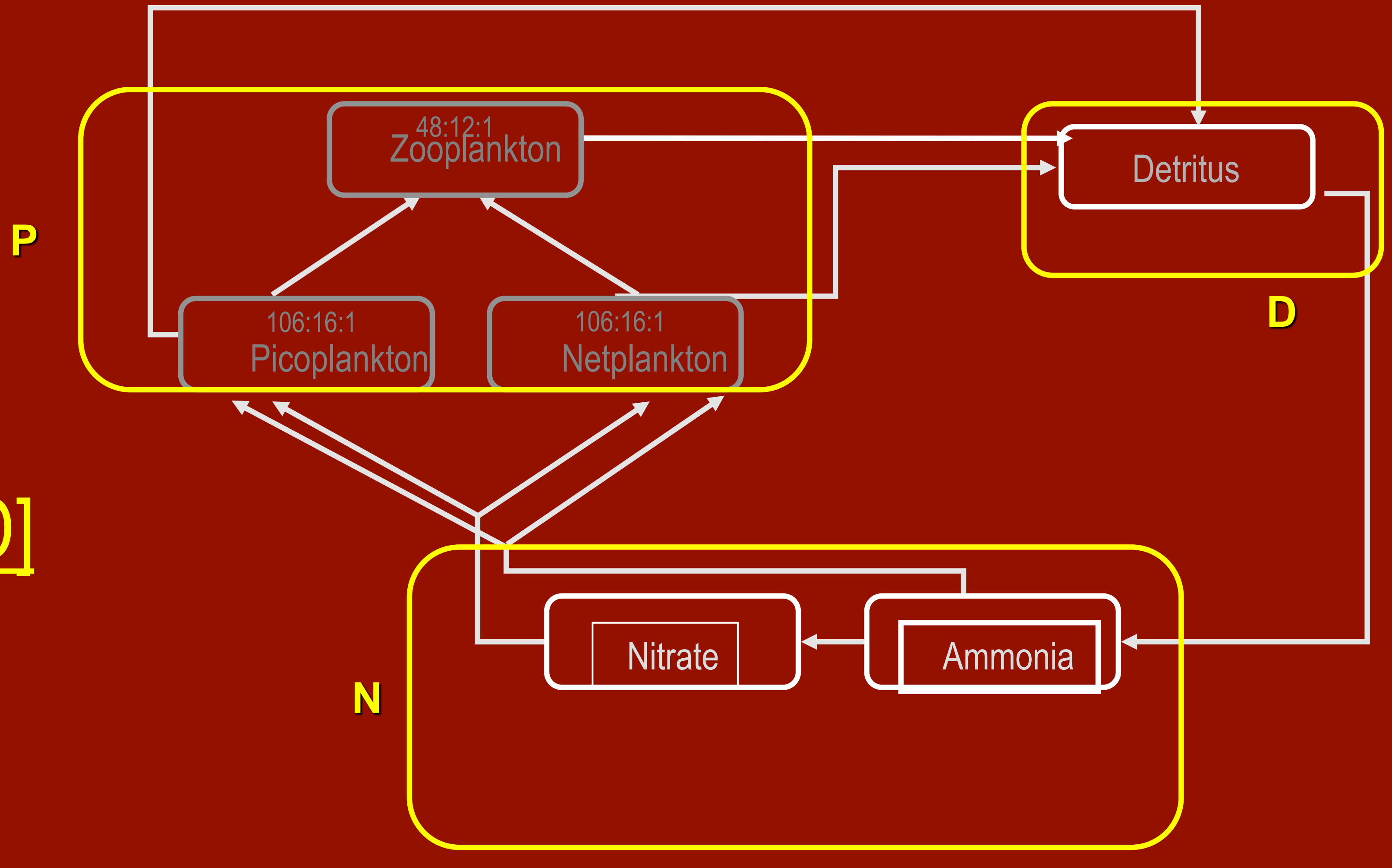
$$q\left(\Theta,\bar{T},\bar{I},..\right)$$

[N,P,D]



The BIOLOGICAL term

$$q\left(\Theta,\bar{T},\bar{I},..\right)$$



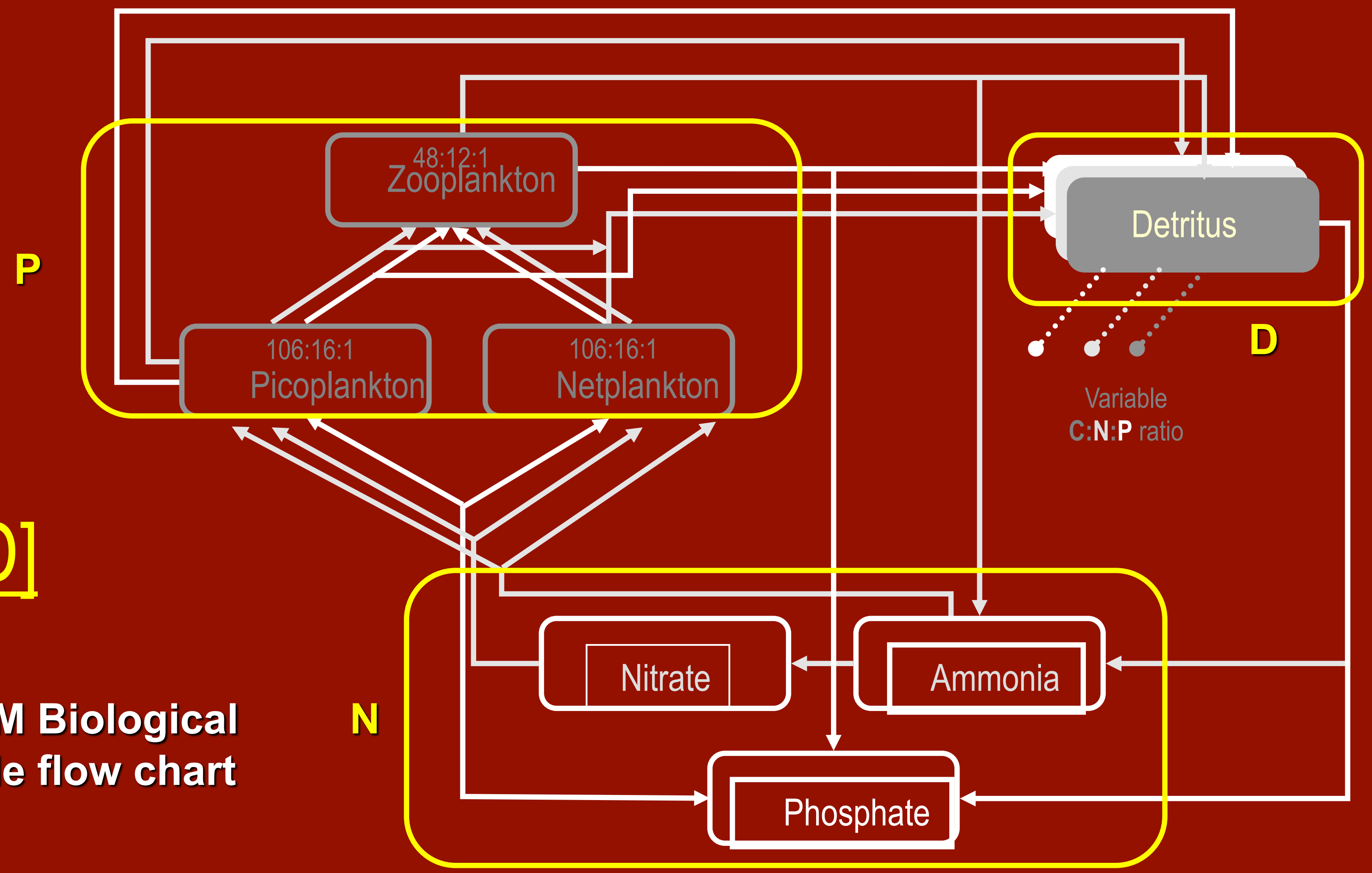
[N,P,D]

The BIOLOGICAL term

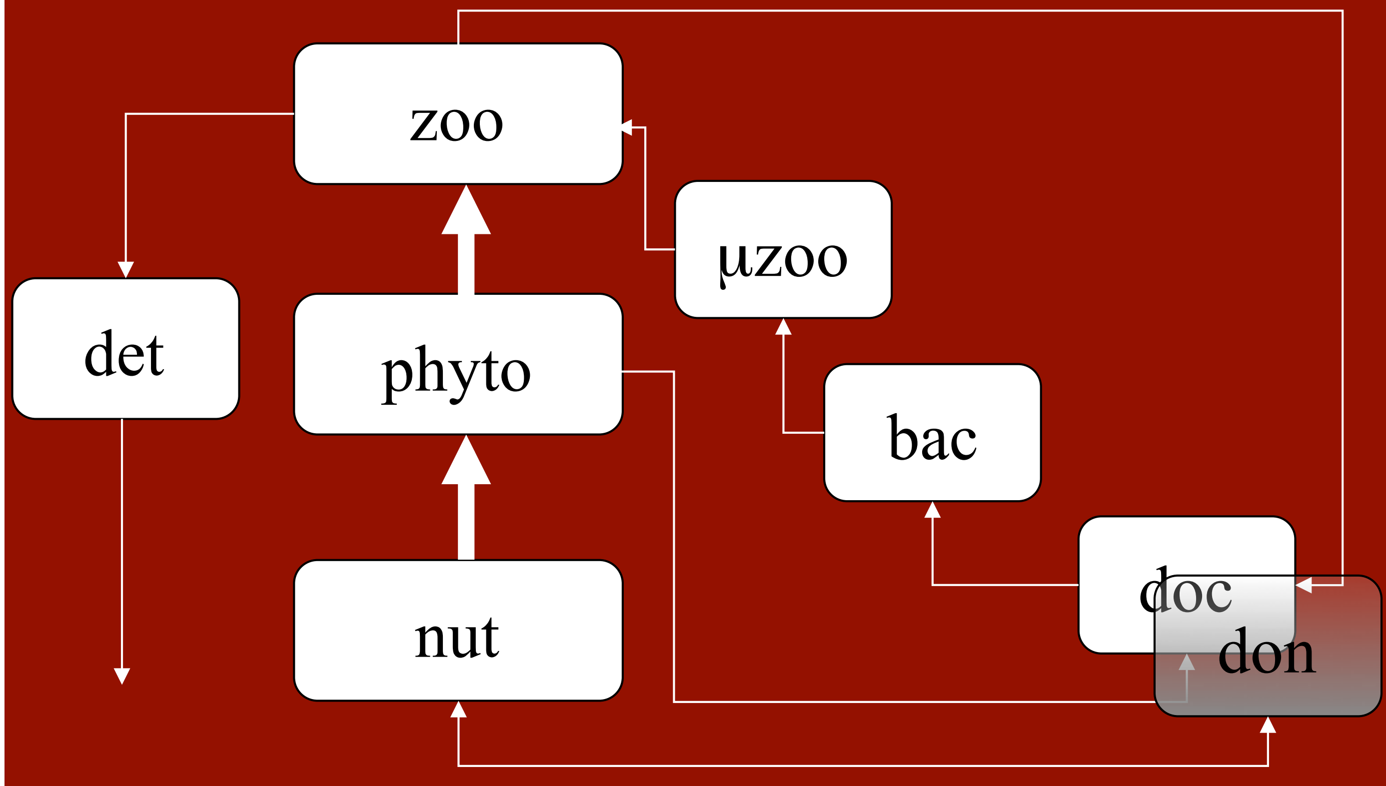
$$q\left(\Theta, \bar{T}, \bar{I}, ..\right)$$

[N,P,D]

ECHYM Biological module flow chart



More complex model: the microbial loop



Bacteria play an important role in trophodynamics, by fuelling enregy matter through higher trophic level.
They decompose DOC, are grazed by microzoo, inturn grazed by mesozoo.

azam, fenchel, thingstand, rassoulzadegan

Severalmodel of increasing complexity ….

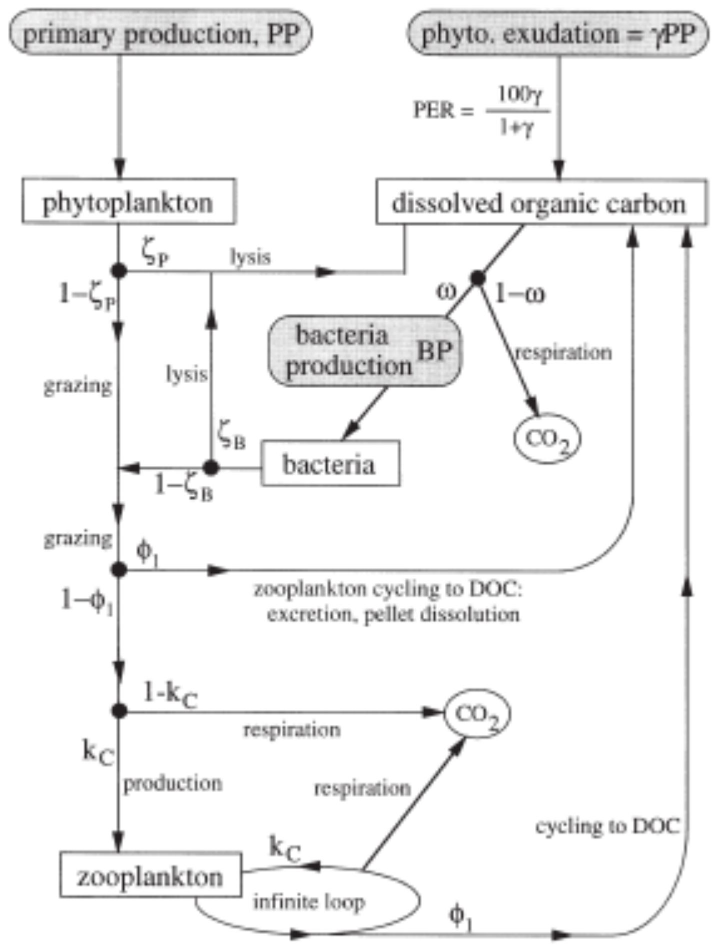


Fig. 1. Flow diagram of the model, illustrating sources, sinks and cycling processes. Parameterization of various flows is indicated. See text for explanation and equations

Andersen & ducklow 01

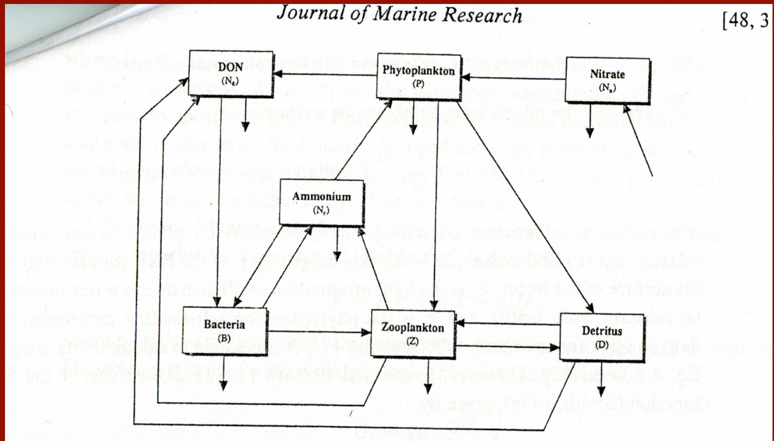
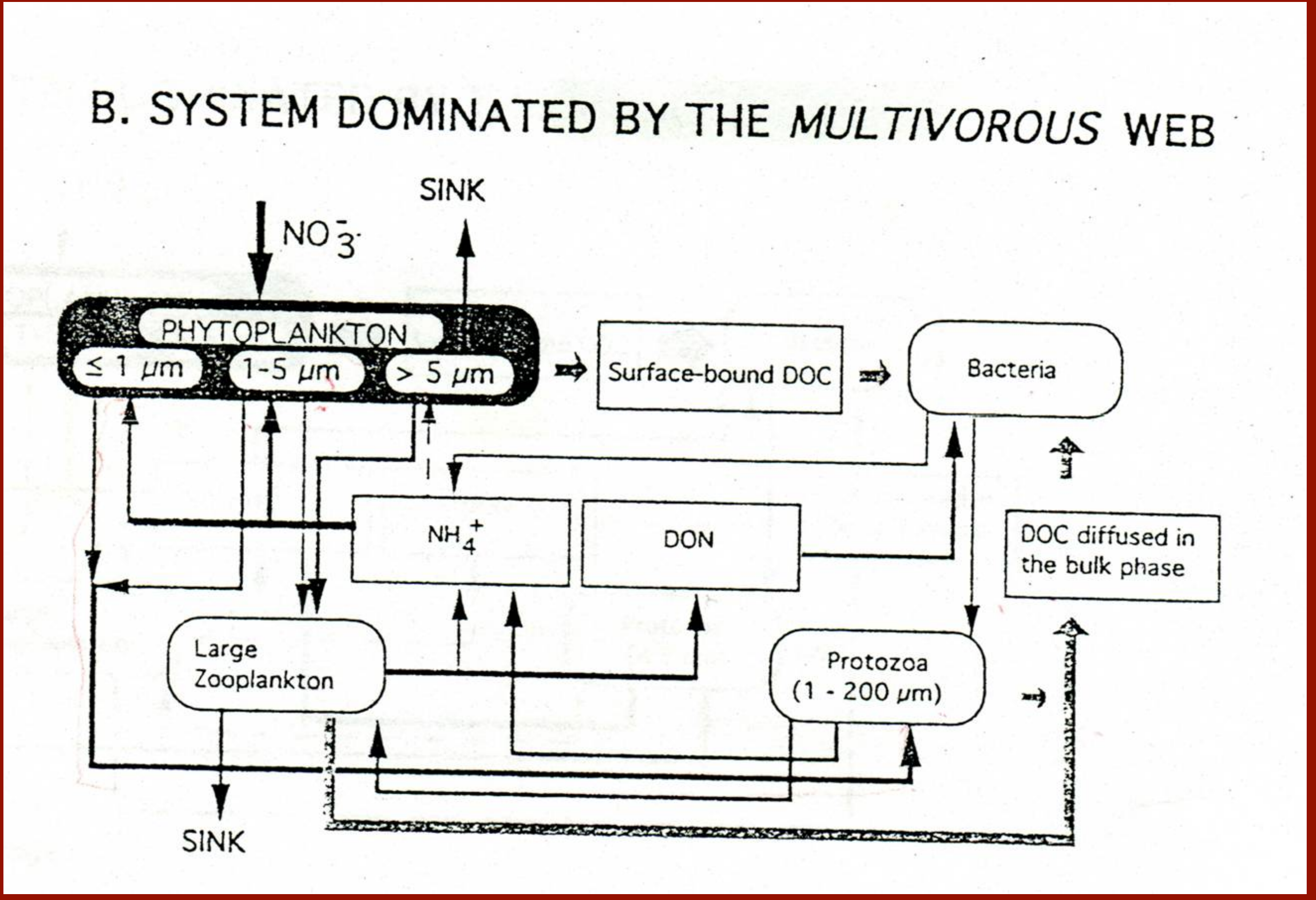


Figure 1. Diagrammatic representation of a nitrogen-based model of mixed layer plankton and nitrogen cycling showing the compartments and the modelled nitrogen flows among compartments and between compartments and the deep ocean.

Fasham 1990

The mistivourous food web (a continuum ..)



Legendere & Rassoulzadegan 1995

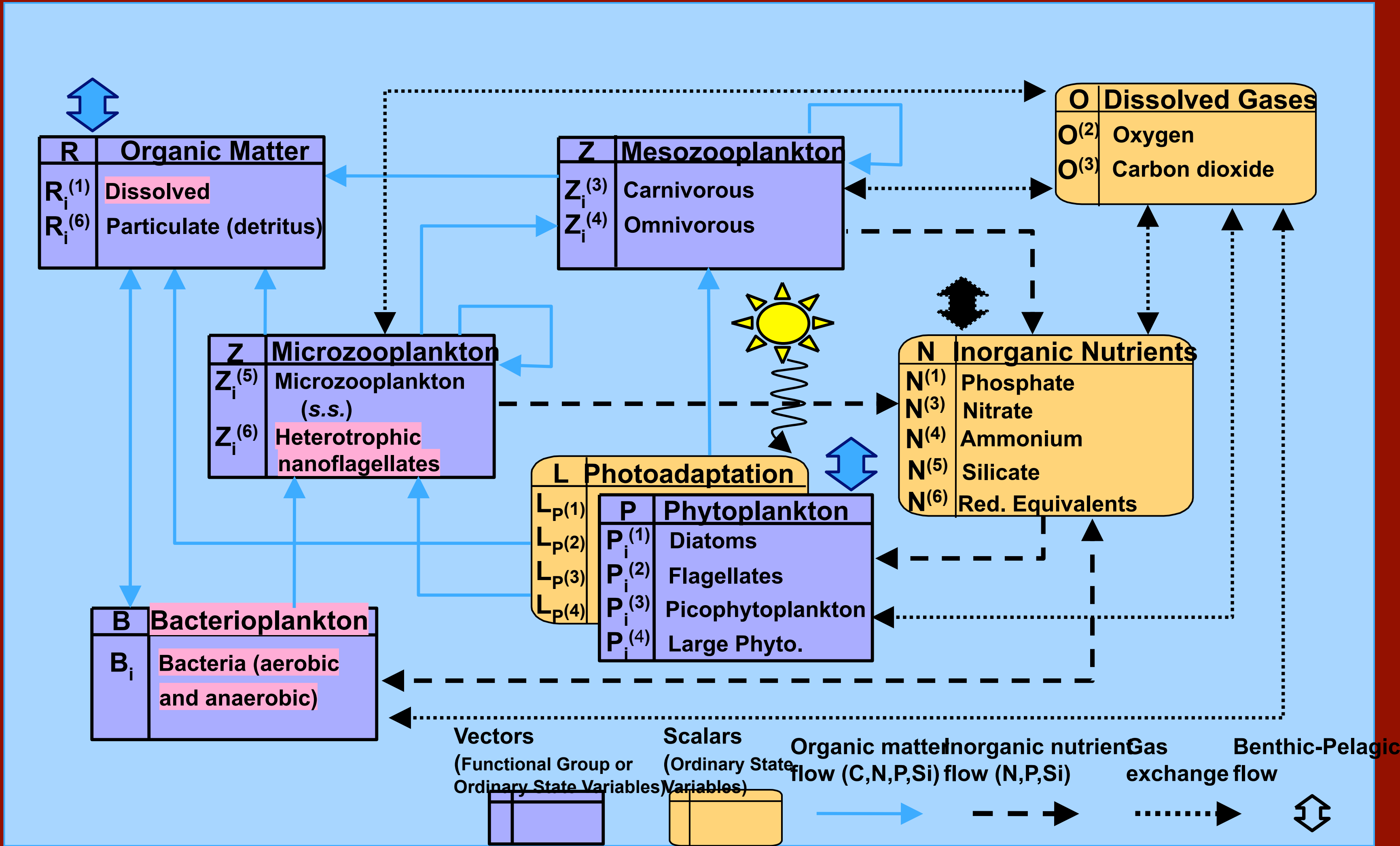
DYNAMIC GREEN MODEL

Approccio Plankton Functional Type PFT

Bacteria	pico-heterotrophs; remineralise dissolved and particulate organic matter
Phyto-plankton	pico-autotrophs; contribute to primary production but not to export of carbon
	N_2-fixers; control total amount of reactive N
	calcifiers; produce more than half the marine carbonate flux, sensitive to pH
	DMS-producers; influence atmospheric sulphur cycle
	mixed; the background biomass of phytoplankton
	silicifiers; contribute to export of carbon to deep ocean
Zoo-plankton	proto; graze on small phytoplankton, control blooms
	meso; graze on all sizes of plankton, produce fast-sinking faecal pellets which export carbon
	macro; graze on all sizes of phyto-plankton and produce fast-sinking faecal pellets

Figure 1. Ten PFTs were identified that need to be simulated explicitly in order to capture important biogeochemical processes in the ocean.

The BIOGEOCHEMICAL FLUX MODEL(PELAGIC)



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HORIZONS

Plankton functional type modelling: running before we can walk?

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Communicating editor: K.J. Flynn

Biogeochemical cycling in marine systems is intimately linked to the activity of specific plankton functional types (PFTs) such as diatoms, coccolithophores and nitrogen fixers, thereby providing a focus for contemporary modelling studies. Incorporating extra complexity beyond simple nutrient-phytoplankton-zooplankton-detritus (NPZD) models is, however, fraught with difficulties: poorly understood ecology; lack of data; aggregating diversity within functional groups into meaningful state variables and constants; sensitivity of output to the parameterizations in question and their physical and chemical environment. Although regional models addressing the seasonal succession of plankton types have achieved some degree of success, predicted distributions of PFTs in global biogeochemical models have thus far been less than convincing. While the continued articulation of detail in

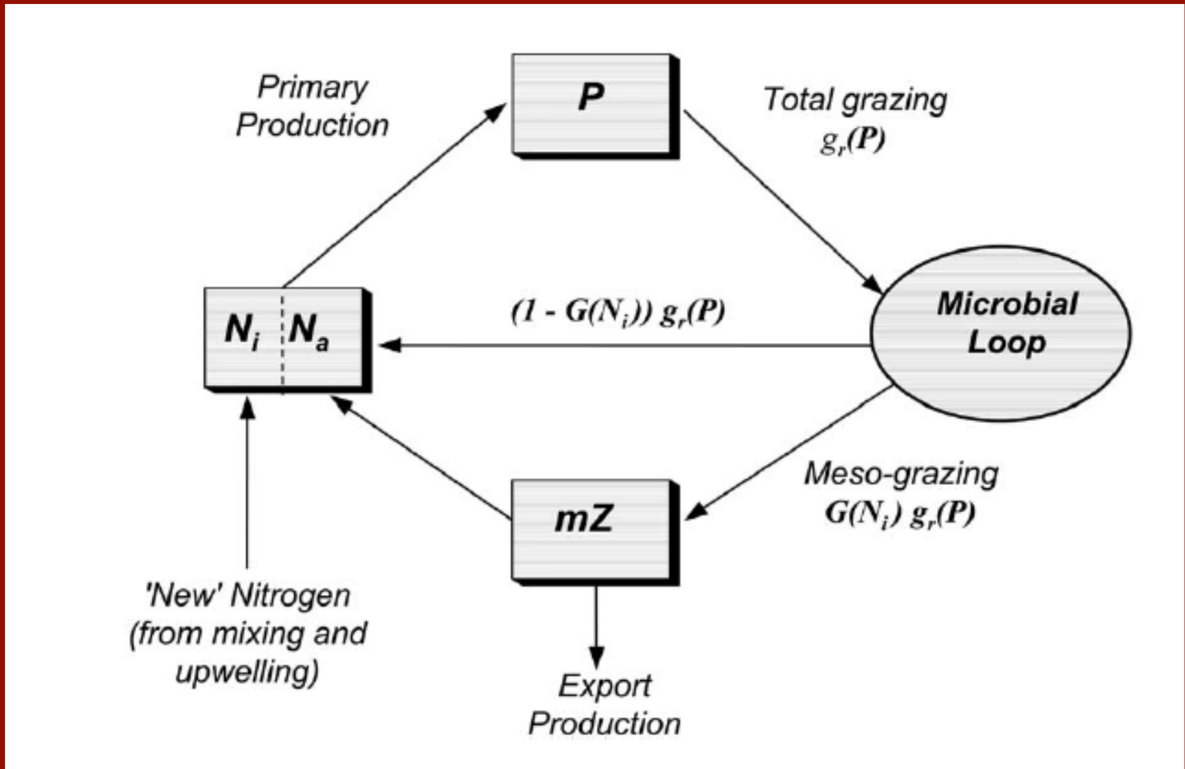
It is relatively straightforward to formulate more complex models to include explicitly different functional groups of phytoplankton, zooplankton and bacteria, and to include regulation by multiple nutrients such a nitrate, ammonium, silica, and iron.

Denman 2003

However, the number of parameters that must be specified from observations increases approximately as the square of the number of compartments and quickly surpasses our ability to constrain them properly from observations. Moreover, ecosystem models often become unstable for small changes in parameter values, and increasing complexity may not lead to increased stability.

Denman 2003

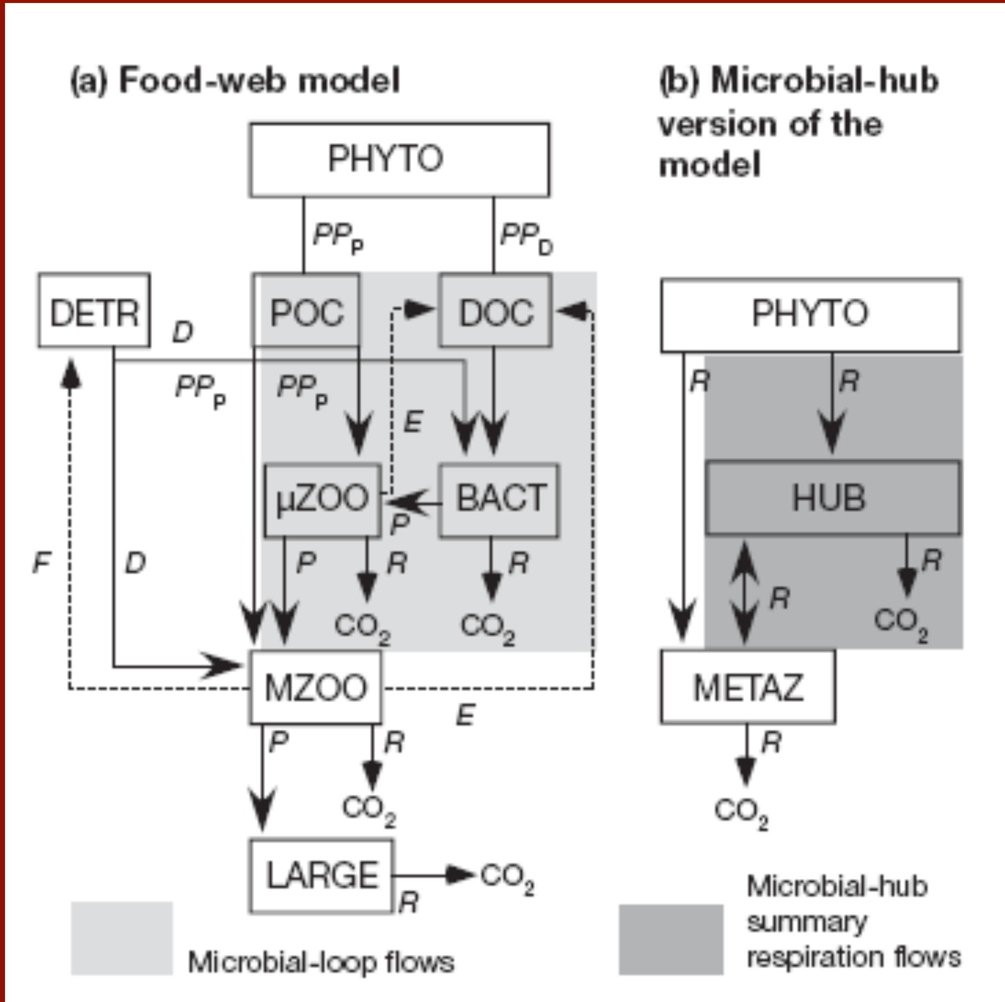
Attempts at simplify (paraemterization) exist ..



Steele 98

implicit treatment of the microbial loop.
the proportion of total grazing that flows directly to mesozooplankton, can vary according to nitrate availability or total phytoplankton

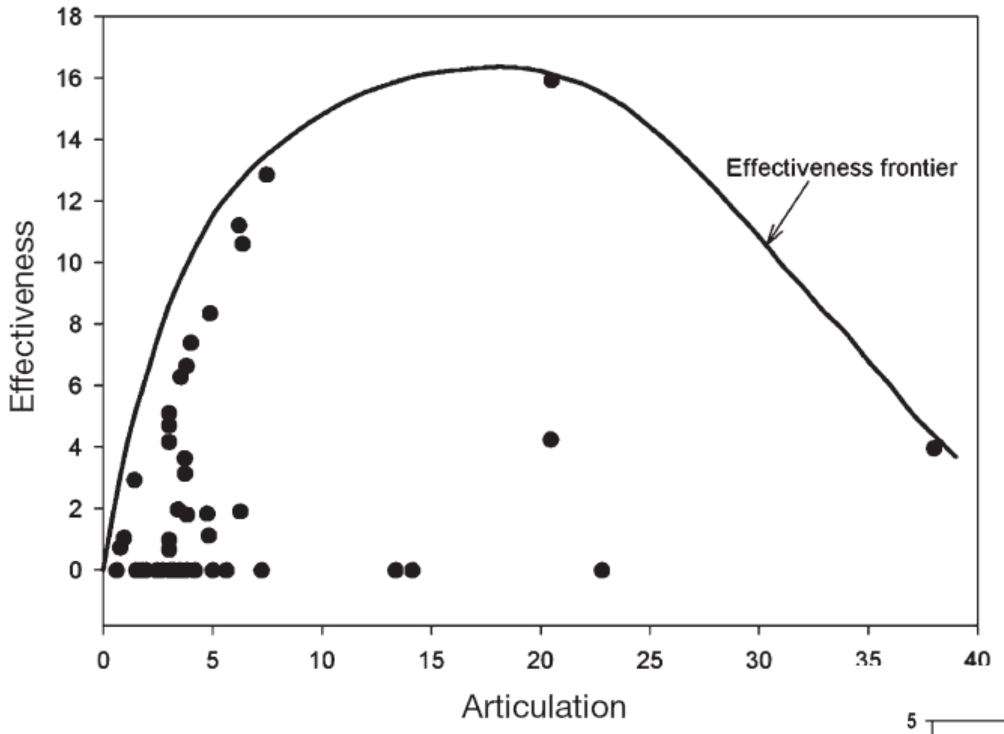
.. but also Armstrong, Denman …



Legendre & RIvkin 2008

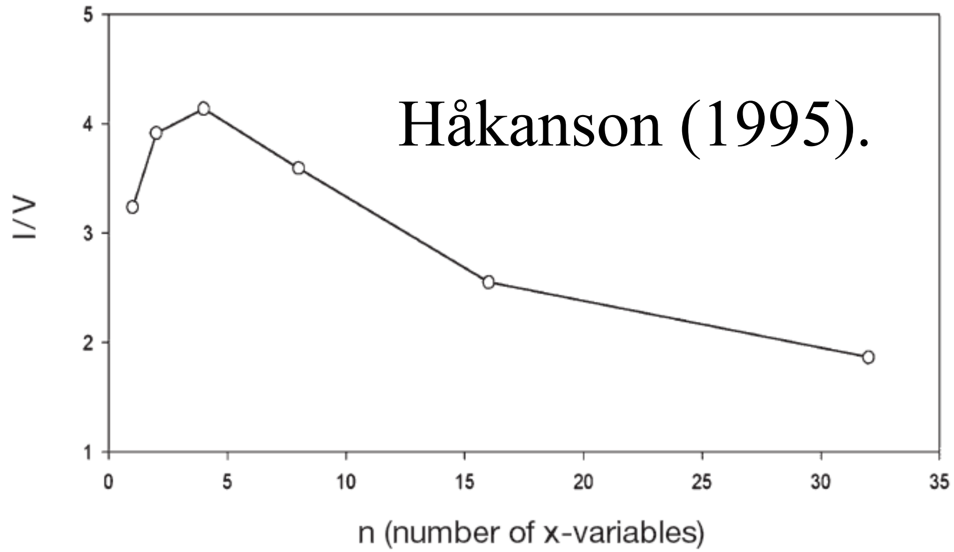
all heterotrophic microbes are grouped together in the HUB, whereas larger heterotrophs are grouped into a metazoan compartment (METAZ)

[… in ogni modello ci sarà sempre qualche grado di disfunzionalità]



Costanza & Sklar (1985)

The main recommendation is that the use of a single 'ultimate' ecosystem model is ill-advised, while the comparative and confirmatory use of multiple 'minimum-realistic' models is strongly recommended (Fulton 2003)



Håkanson (1995).

are simple models that simple?

$$q\left(\Theta, \bar{T}, \bar{I}, ..\right)$$

	riareation	Degradazione aerobica detrito	Fotosintesi assimilazione nutriente	Mortalità fito	Respirazione fito
oxygen	riareazione	-degradazione	fotosintesi		
Detrito		-degradazione		mortalità	
Plancton			fotosintesi	- mortalità	- respirazione
nutriente		degradazione	-fotosintesi		respirazione

A closer look to the BIOLOGICAL term

are simple models that simple?

$$q\left(\Theta,\bar{T},\bar{I},..\right)$$

	riareation	Detitus degradation	Fotosintesi assimilazione nutriente	Mortalità fito	Respirazione fito
Oxygen	riareazione	-degradazione	fotosintesi		
detritus		-degradazione		mortalità	
plankton			fotosintesi	- mortalità	- respirazione
nutrient		degradazione	-fotosintesi		respirazione

A closer look to the BIOLOGICAL term

are simple models that simple?

$$q\left(\Theta, \bar{T}, \bar{I}, ..\right)$$

	riareation	Detitus degradation	Photosynthesis and nutrient assimilation	Phyto mortal	…
oxygen	riareazione	-degradation	photosynthesis		
Detritus		- degradation		mortality	
Plankton			photosynthesis	- mortalità	- respirazione
nutrient		degradation	-photosynthesis		respirazione

A closer look to the BIOLOGICAL term

are simple models that simple?

$$q\left(\Theta, \bar{T}, \bar{I}, ..\right)$$

	riareation	Detitus degradation	Photosynthesis and nutrient assimilation	Phyto mortal	…
oxygen	$-k_{rear}(DO-DOsat)$	$-k_{dec}D$	$K\mu_{max}\frac{N}{N+k}\frac{I}{I_o}\exp\left\{1-\frac{I}{I_o}\right\}A\exp\left(-\frac{B}{T}\right)F$		
Detritus		$-k_{dec}D$			
Plankton					
nutrient			$\mu_{max}\frac{N}{N+k}\frac{I}{I_o}\exp\left\{1-\frac{I}{I_o}\right\}A\exp\left(-\frac{B}{T}\right)F$	$-k_m F$	
		$k_{dec}D$	$-\mu_{max}\frac{N}{N+k}\frac{I}{I_o}\exp\left\{1-\frac{I}{I_o}\right\}A\exp\left(-\frac{B}{T}\right)F$	$+k_m F$	

A closer look to the BIOLOGICAL term

PHYTO GROWTH (PHOTOSYNTESIS)

MULTIPLICATIVE MODEL

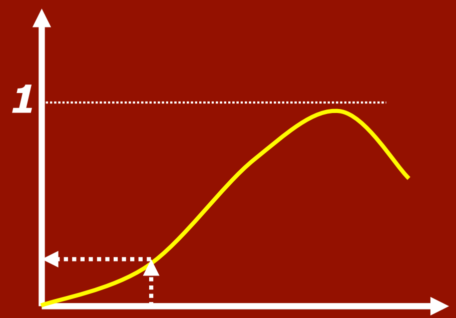
Photosyntheis varies with environmental factors.

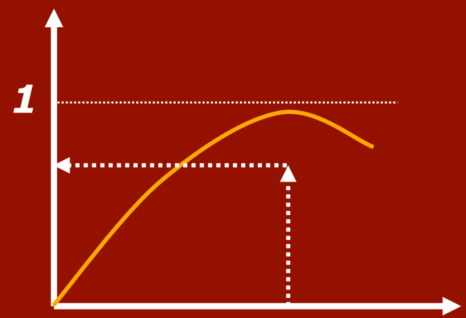
It is max at optimal level of I, T, & Nut (N,P)

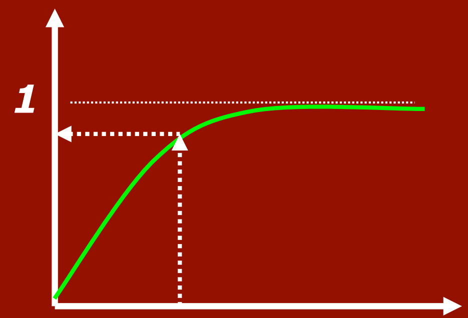
$$\mu = \mu(I, T, N) = \mu_{max} f(N) f(P) f(I) f(T)$$

Growth rate = max value * adimensioanl factor ranging from 0 to 1.
Each factor defines the extent of growth limitation because of suboptimal environemental conditions

F(T) F(I) F(N)

Kmax * 

* 

* 

Kmax * LASSITER * STEELE * MONOD

equations in the water quality submodel (mass balances)

$$\frac{d[Phy]}{dt} = growth_{Phy} - resp_{Phy} - mort_{Phy} - grazing - sink_{Phy}$$

$$\frac{d[Zoo]}{} = Keff_{\ } \cdot grazin$$

$$\frac{d[NH_4^+]}{} = -r \cdot growth \cdot \frac{[NH_4^+]}{} + r \cdot \{resp$$

$$\frac{d[NO_3^-]}{dt} = -r_{nc} \cdot growth_{phy} \cdot \frac{[NO_3^-]}{N_{tot}} + nitrific - denitrif$$

$$\frac{d[PO_4^{3-}]}{dt} = -r_{pc} \cdot growth_{Phy} + r_{pc} \cdot \{resp_{Phy} + excret_{Zoo}\} + decay_{DetP} + decay_{SedP}$$

$$\frac{d[DetC]}{dt} = (1 - Keff_{Zoo}) \cdot grazing + mort_{Zoo} + mort_{Phyto} - decay_{DetN} - sink_{DetC}$$

$$\frac{d[DetN]}{} = r \cdot \{(1 - Keff_{\ }) \cdot grazing + m$$

$$\frac{d[DetP]}{dt} = r_{pc} \cdot \{(1 - Keff_{Zoo}) \cdot grazing + mort_{Phy} + mort_{Zoo}\} - decay_{DetP} - sink_{DetP}$$

$$\frac{d[SedC]}{dt} = sink_{DetC} + sink_{Phy} - decay_{SedC}$$

$$\frac{d[SedN]}{dt} = sink_{DetN} + r_{nc} \cdot sink_{Phy} - decay_{SedN}$$

$$\frac{d[SedP]}{} = sink + r$$

$$\frac{d[Oxy]}{} = r \cdot [growth - resp - decay - de$$

$growth = GP \cdot \{F$

$F = \left[(T_{max} - T_m) \right]^{\alpha}$

$F_N = N_{tot} / [K_N + N_{tot}]$

$N_{tot} = [NH_4^+] + [NO_3^-]$

$F_P = [PO_4^{3-}] / [K_P + [PO_4^{3-}]]$

$T = min$

$F \quad I_k$

$F = [Oxy]/[$

$$I_k = I_{sun} \cdot e^{-\left(Kest \cdot k + \int_0^k Kself_{Phy} \cdot [Phy] dz\right)}$$

$decay = Kdec$

$$denitrif = ([NO_3^-] \cdot Kdeni - 0.119) \cdot Q_{10}$$

..but alternative way to combine limitations was proposed

MULTIPLICATIVE

$$\mu = \mu(I, T, N) = \mu_{max} f(N) f(I) f(T)$$

MINIMUM (Liebig)

$$\mu = \mu_{\max} \min\{f(N), f(I), f(T)\}$$

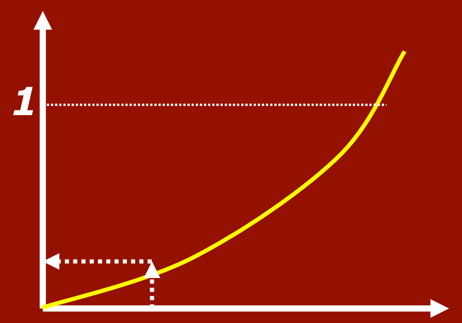
'mixed'

$$\mu = \mu_{\max} f(I) f(T) \min\{f(N), f(P)\}$$

..as well as differnet ways to describe limitation

Example of f(T)

no hinibition, no limit



van't hoff

$$\frac{d\ln k}{dt} = \frac{\Delta H}{RT^2}$$

$$\ln\left(\frac{k_2}{k_1}\right) = \frac{-\Delta H}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

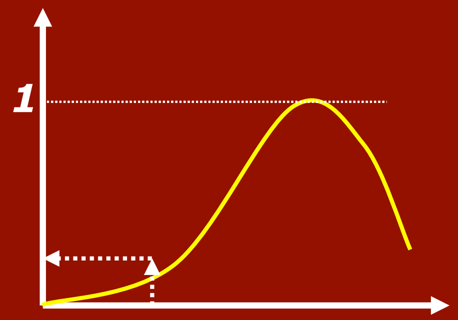
Arrenhius (Q10)

$$k = Ae^{-E_a/RT}$$

$$f(T) = \theta^{(T-T_0)}$$

… non normalized to 1 !!!

Example of f(T)

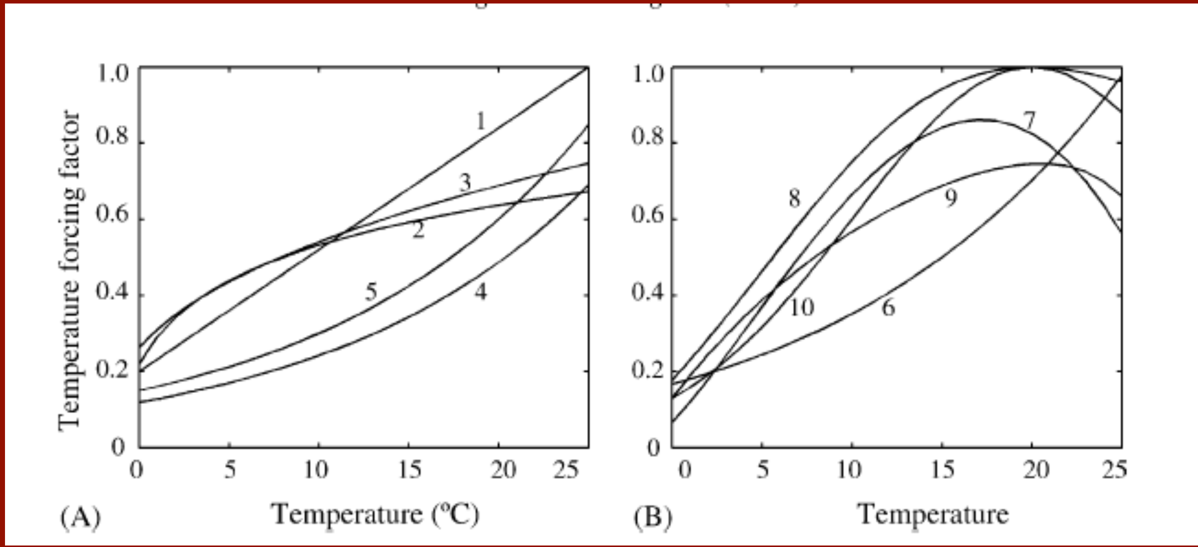


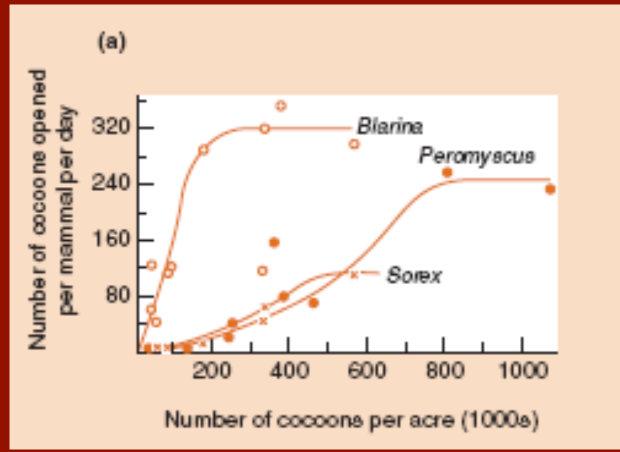
Inibhition

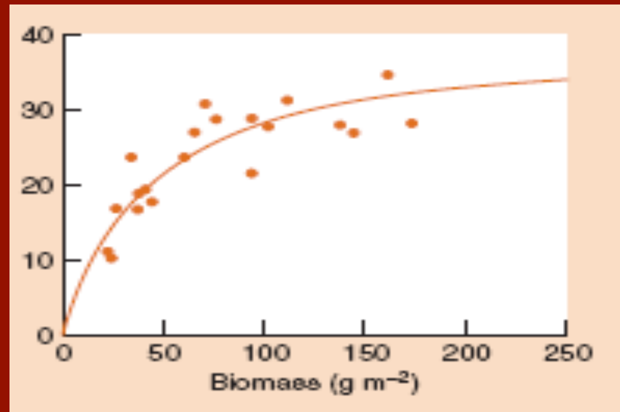
Normalized to 1

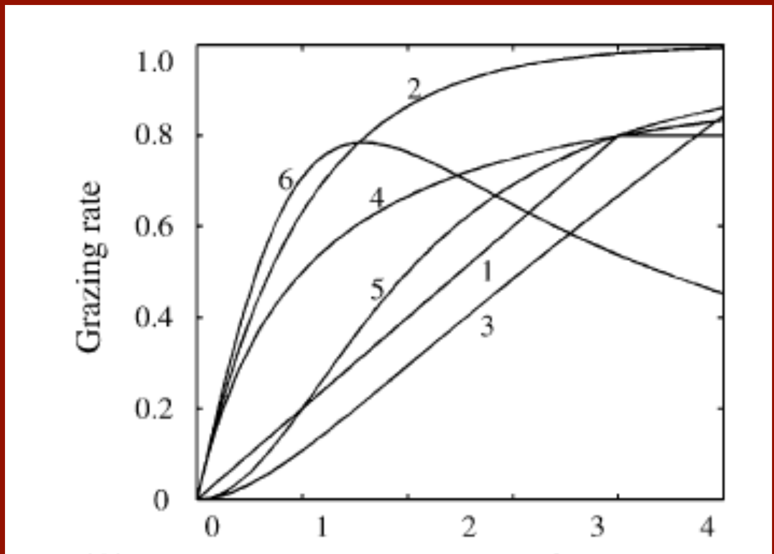
Lassiter e Kearns (74)

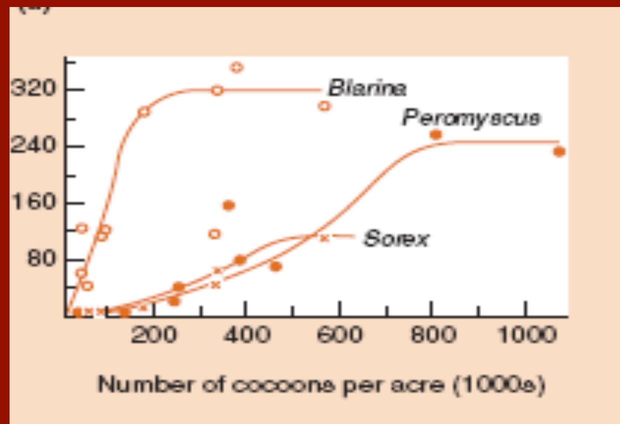
$$f(T) = \left[\frac{(T_{\max} - T) -}{(T_{\max} - T_{opt})}\right]^{\alpha(T_{\max} - T)} e^{\alpha(T - T_{opt})}$$



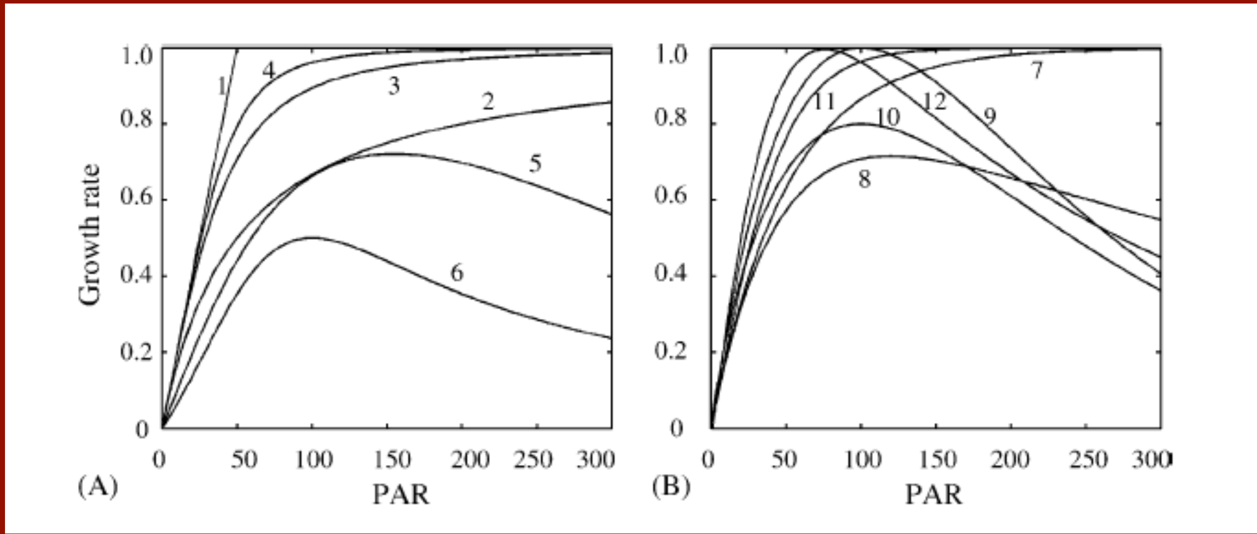




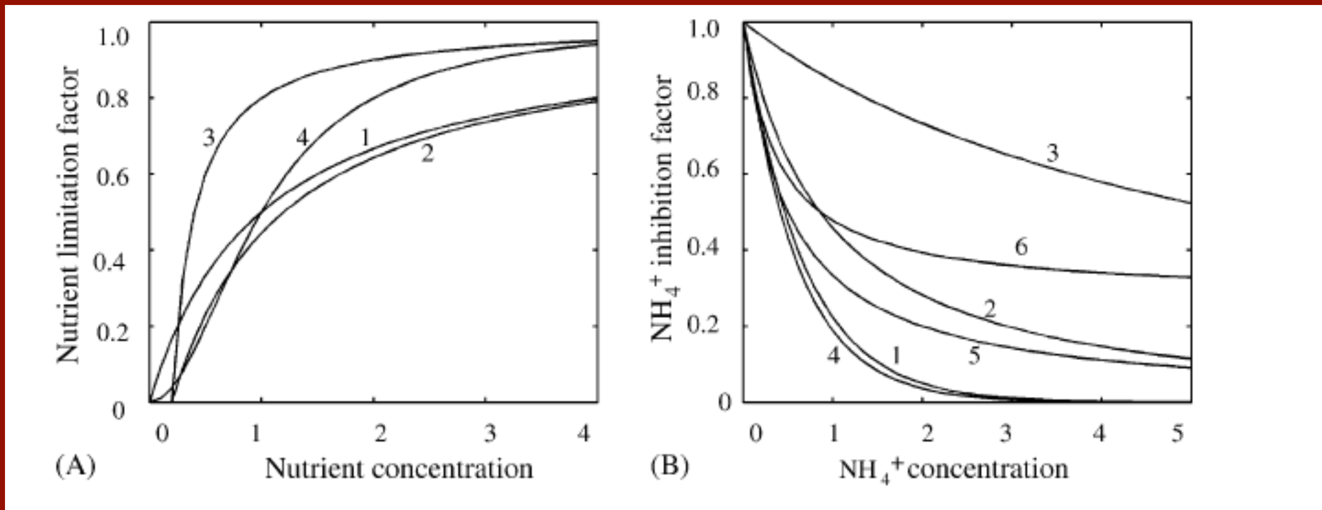




Mostly empirical, with a posteriori ‘phyisological’ derivation



Growth rate
PAR
(A)
(B)
1.0
0.8
0.6
0.4
0.2
0
0
50
100
150
200
250
300
1
2
3
4
5
6
7
8
9
10
11
12



Nutrient limitation factor
Nutrient concentration
(A)
NH_4^+ inhibition factor
NH_4^+ concentration
(B)
1.0
0.8
0.6
0.4
0.2
0
1
2
3
4
5
6

28 parametri

GPmax	0.18 [h-1]	max growth rate for phyto (optimal values of T , I and nutrients)
KmPho	0.006 [h-1]	death rate for phytoplankton
KrPhy	0.003 [h-1]	respiration rate for phytoplankton
KN	0.05 [mg N/L]	halfsaturation constant for nitrogen assimilation
KP	0.01 [mg P/L]	halfsaturation constant for phosphorus assimilation
Topt	27 [° C]	optimal temperature for phytoplankton growth
Tmaxx	41 [°C]	inhibition temperature for phytoplankton growth
?	0.15 [°C-1]	Lassiter e Kearnes exponential coefficient
rnc	0.15 mg N/mg C	N/C ratio in phytoplankton (Redfield ratio)
rpc	0.023 mg P/mg]	N/C ratio in phytoplankton (Redfield ratio)
Light parameters		
Iopt	50000 [lux]	optimal light for phytoplankton growth
KselfPhy	4. [mg C-Phy/L]	self-shading coefficient for phytoplankton
Kest	1.0 [m-1]	shading coefficient
Parameters of zooplankton dynamic		
Kgr	0.04 [h-1]	max grazing rate
Kgphyto	1. [mg C-Fito/L]	halfsaturation constant for grazing formulation
KmZoo	0.006 [h-1]	death rate for zooplankton
KeffZoo	0.5 [dimensionless]	grazing efficiency
KeZoo	0.002 [h-1]	excretion rate for zooplankton
Parameters of nitrogen dynamic		
Knit	0.0043 [h-1]	nitrification rate at 20°C
Kdenii	1.6 [mg NO3-/l/h]	denitrification rate
Parameters of sediment and detritus dynamics		
KdecDet	0.0048 [h-1]	decay rate of organic detritus at 20° C

…….

NO DEFAULT OPTIONS:
YOU HAVE TO KNOW WHAT YOU ARE DOING

3) ..many models exist..

Increasing complexity →

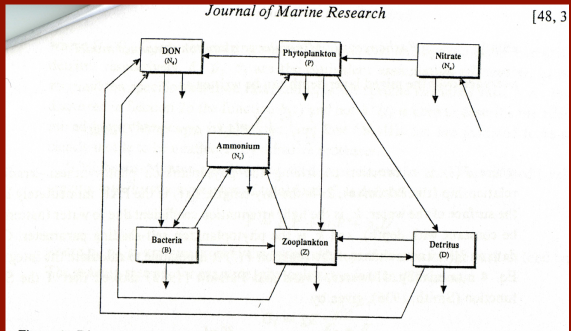
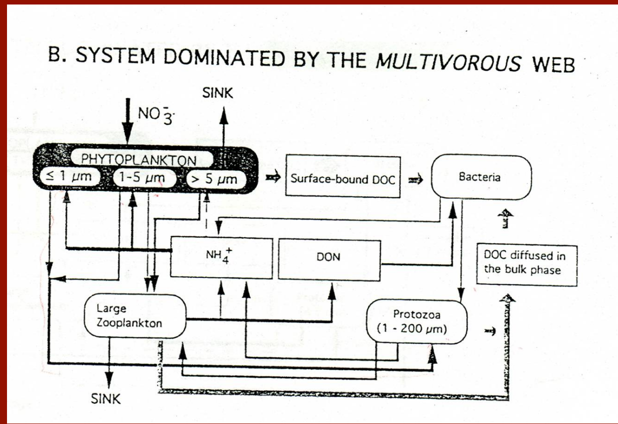


Figure 1. Diagrammatic representation of a nitrogen-based model of mixed layer plankton and nitrogen cycling showing the compartments and the modelled nitrogen flows among compartments and between compartments and the deep ocean.

Fasham, 1990



Legendere & Rassoulzadegan, 1998

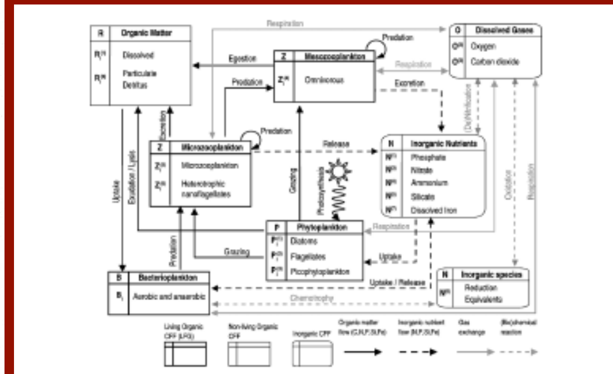
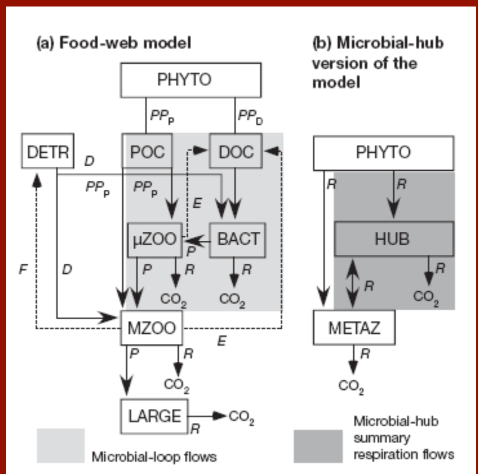


Fig. 3. Scheme of the state variables and pelagic interactions of the biogeochemistry model. Living (organic) Chemical Functional Families (CFF) are indicated with bold-line square boxes, non-living organic CFFs with thin-line square boxes and inorganic CFFs with rounded boxes (modified after Blackford and Radford, 1995).

ERSEM/BFM/PFT (2006)

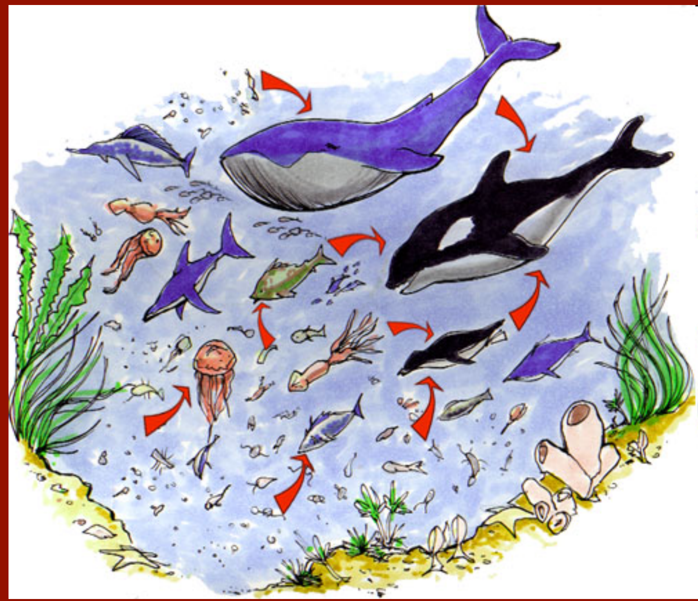


Rivkin & Legendre, 2008

How complex shuold a model be ?

(how simple can a model be) ?

4) ...nature is not be simple...

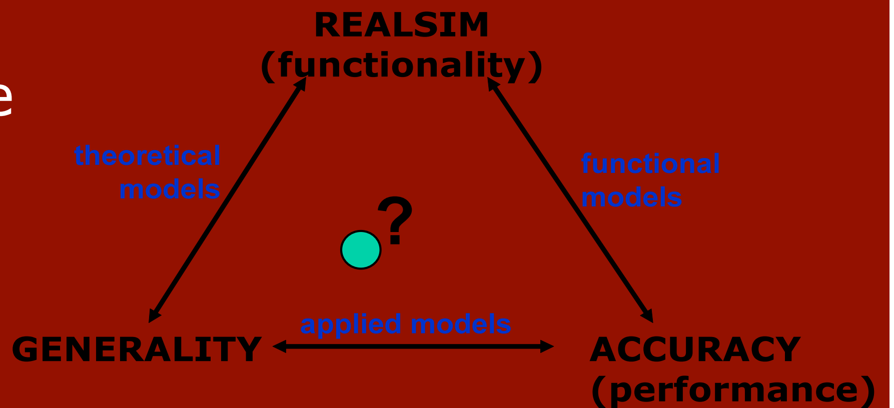


.. And granted that oceanograpic models are disfunctional:

What can we gain in using more functional (but also more complex) representation?

is it worth?

'Keep the model as simple as possible & as compex as needed'?



Calibration and parameters identifiability

Not all paraemters can be identified by calibration
(fitting vs experiemtnal observation)

problems are:
- over and/or underdetermination (# eqs vx # unknown)
- no exact solution
- existence of multiple optimal solutions

(there are more than one combianation of parameters which give the same fit. This is WITHIN equations and cannot be solved)

$$f_N = \boxed{V_m} \frac{n}{n + \boxed{h}}$$